Water vapour profiles by ground-based FTIR Spectroscopy: study for an optimised retrieval and its validation

by M. Schneider, F. Hase, and T. Blumenstock

1. Inversion on a logarithmic scale, why ?
2. Error characterization (… towards an optimal strategy for UT H_2O retrieval)
3. 7-year record of water vapour above Izaña observatory
4. Summary and outlook

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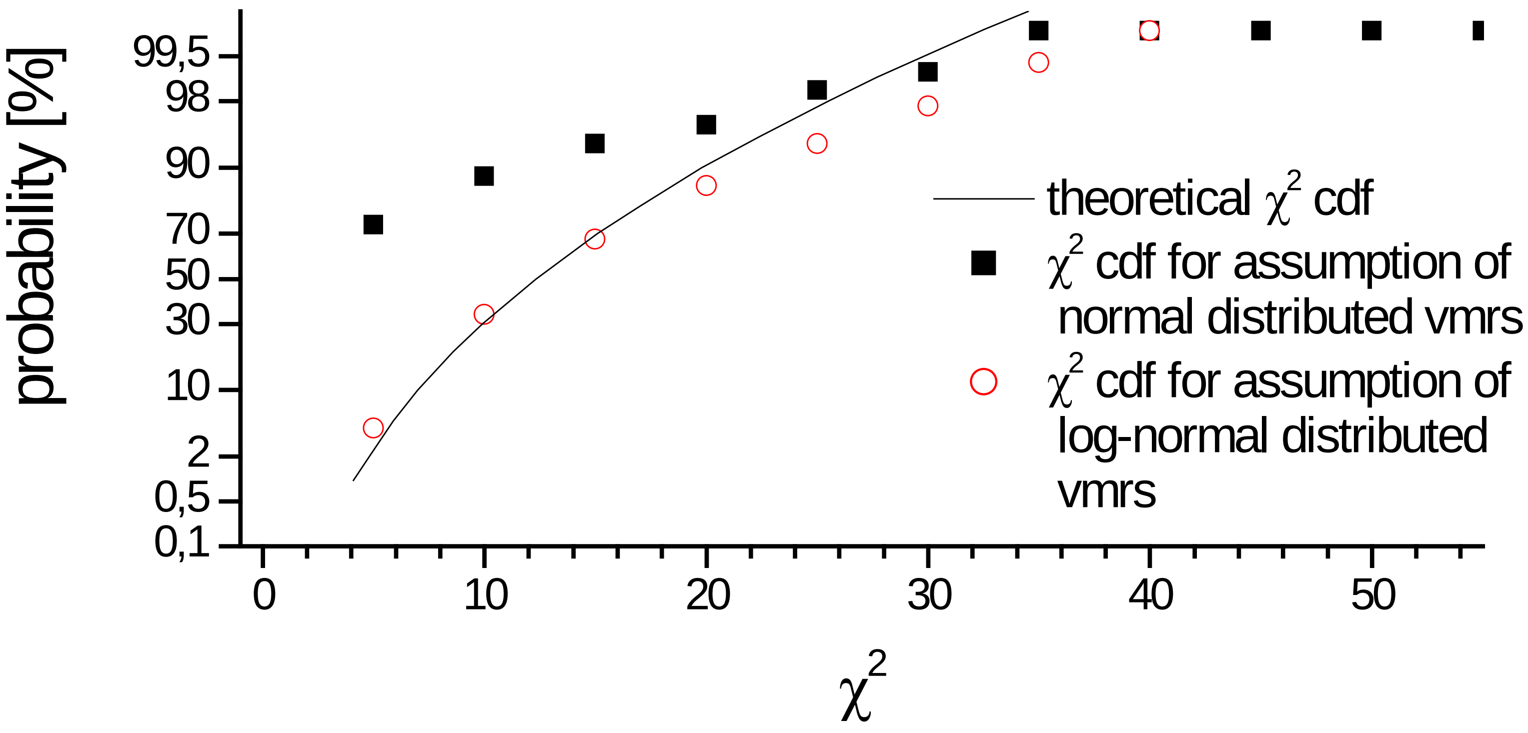
Examination of a-priori distribution. χ^2 test checks for a normal distribution:

$$\chi^2 = (x - x_a)^{\mathrm{T}} \mathrm{S}_a^{-1} (x - x_a)$$



The cost function

$$\sigma^{-2}(y-\mathrm{K}x)^{\mathrm{T}}(y-\mathrm{K}x)+(x-x_a)^{\mathrm{T}}\mathrm{S}_{\mathrm{a}}^{-1}(x-x_a)$$

is only correctly posted if state vector is transformed on a logarithmic scale !

On a linear scale a wrong a-priori distribution is assumed !
Then the term

$$(x-x_a)^{\mathrm{T}}\mathrm{S}_{\mathrm{a}}^{-1}(x-x_a)$$

provides for an overestimation of small x and an underestimation of large x !

Error estimation is performed by a „Monte Carlo“ method. Analytic error estimation like proposed by Rodgers (1990) is not appropriate due to non-linearities.

1. Forward calculation of assumed H_2O profile
2. Introducing of errors (measurement noise, temperature profile, ILS, spectroscopic parameter, …)
3. Inversion of the simulated spectra

This „Monte Carlo“ error estimation works only if we apply a large ensemble of H2O profiles, which obey the real H_2O statistics ! We apply 500 ptu-sonde measurements of the years 1999 and 2000.

Errors are commonly presented as a mean (systematic error) and variance (random error).

Here we present them in a more general manner: by least squares fits

→ difference of regression curve from diagonal: offset + slope of regression line (mean + sensitivity as systematic error)

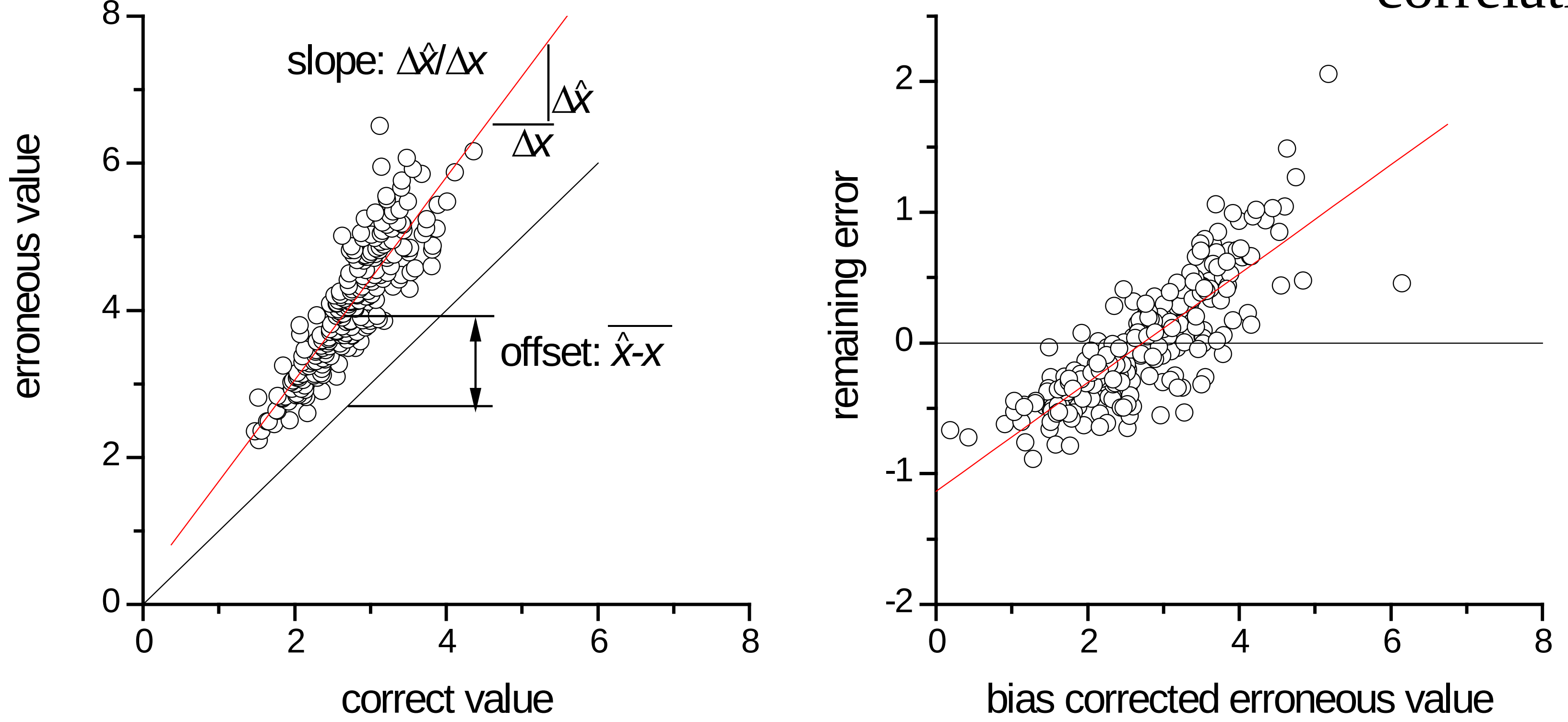
→ scattering around the regression curve (residual variance as random error):

$$\frac{\sigma_{\varepsilon\_reg}}{\sigma_{\hat{x}}} = \sqrt{1-\rho^2}$$

Error estimation by means of linear least squares fit

Why? — there are two kind of systematic errors:

1. mean error (bias)
2. sensitivity error (slope≠1 or no linear correlation)



In the following the errors of lower, middle, and upper tropospheric H_2O are

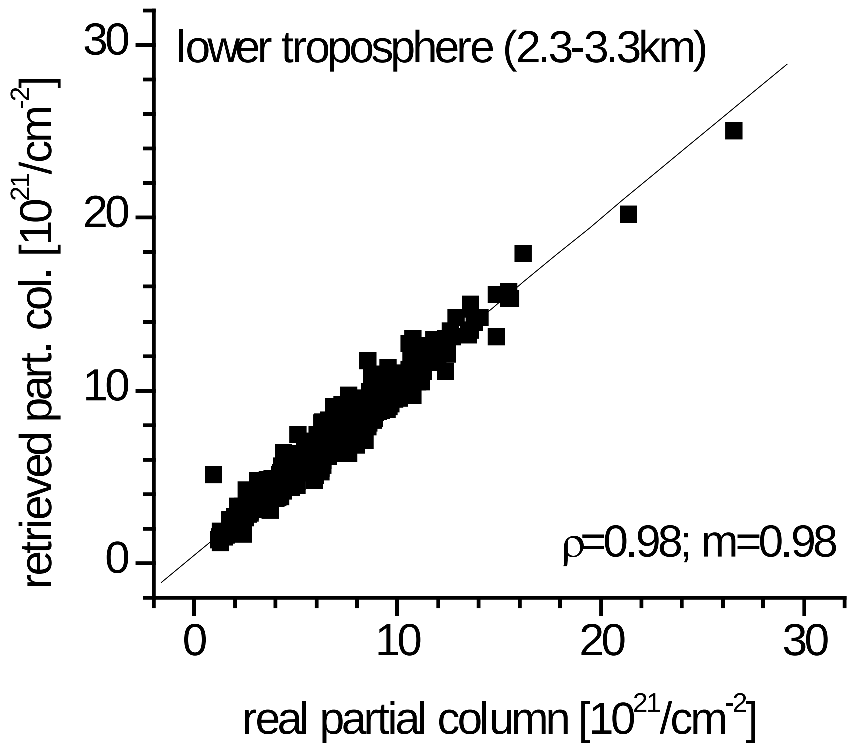
1. estimated by Monte Carlo simulations

and

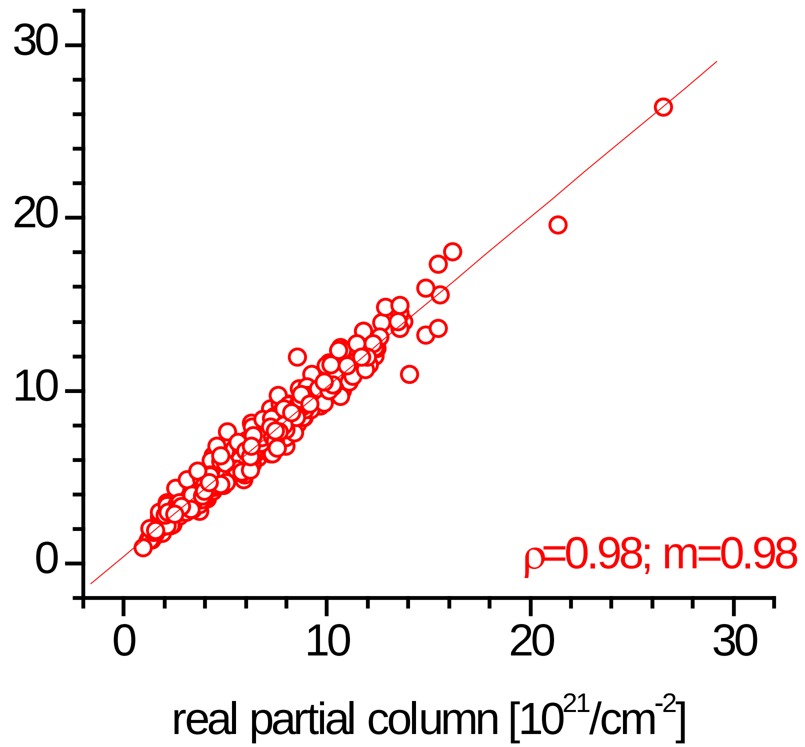
2. validated by comparing H_2O from FTIR measurements with daily ptu-sondes

Estimation of total FTIR error (2.3-3.3km):

linear scale

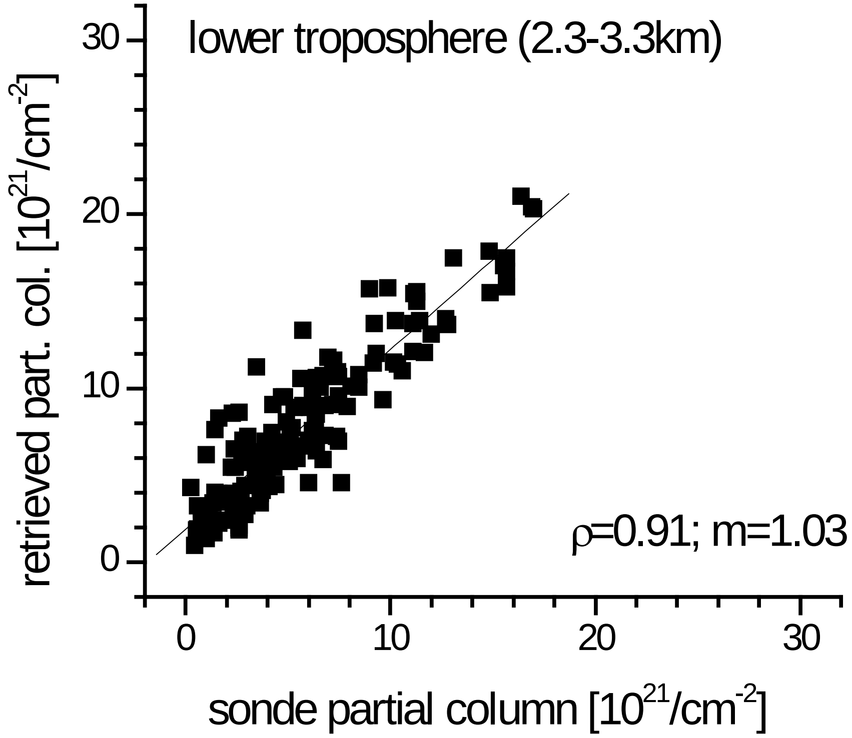


logarithmic scale

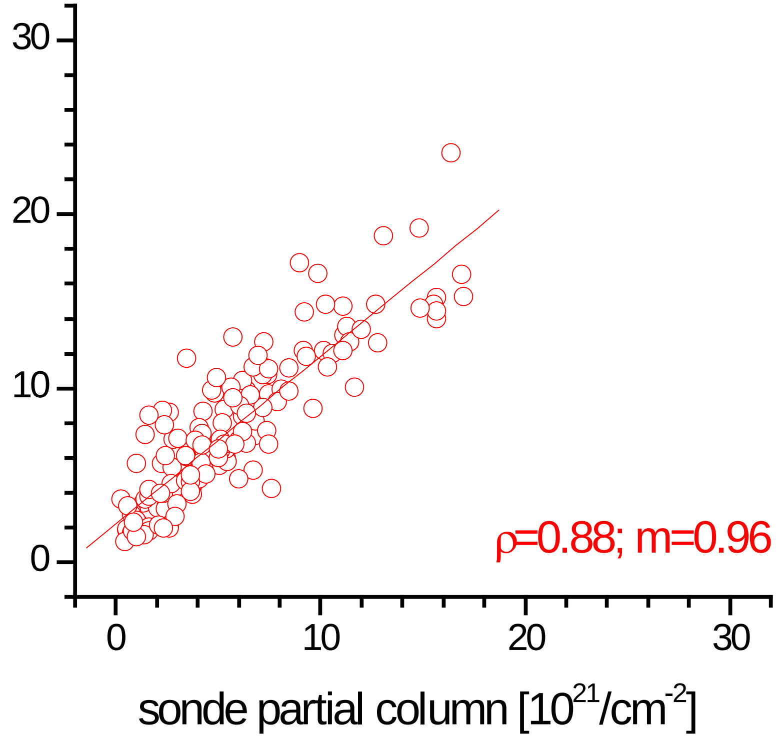


FTIR vs. ptu-sondes at 2.3-3.3km. Problem: detection of different regions (FTIR: boundary layer; sonde: free troposphere)

linear scale

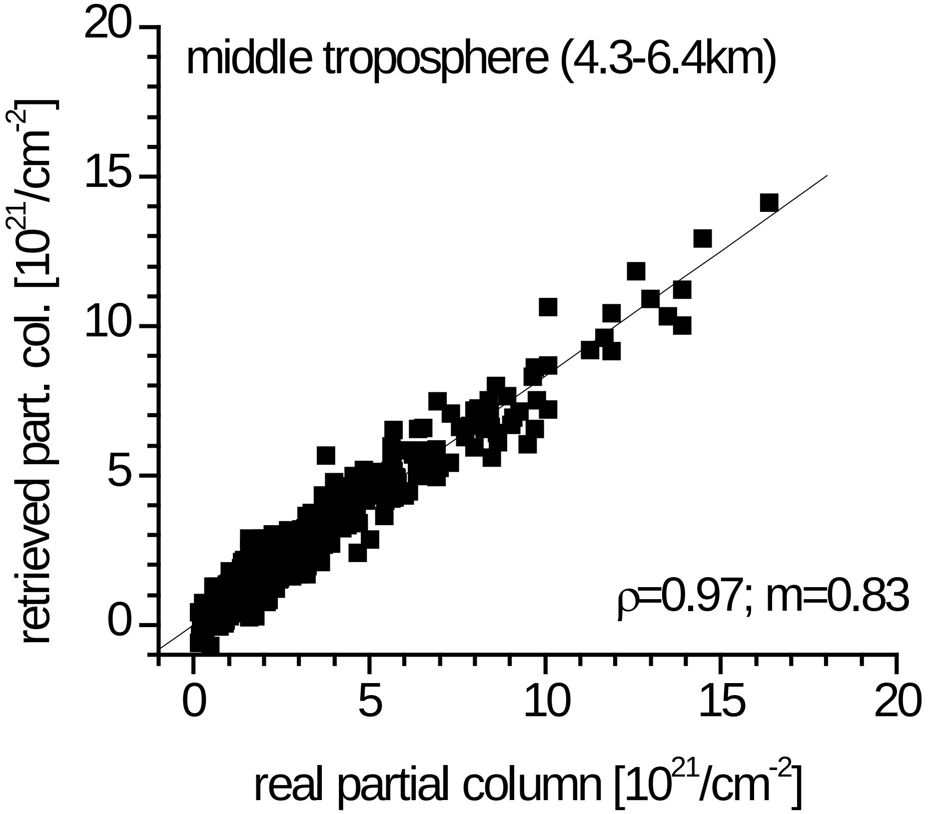


logarithmic scale

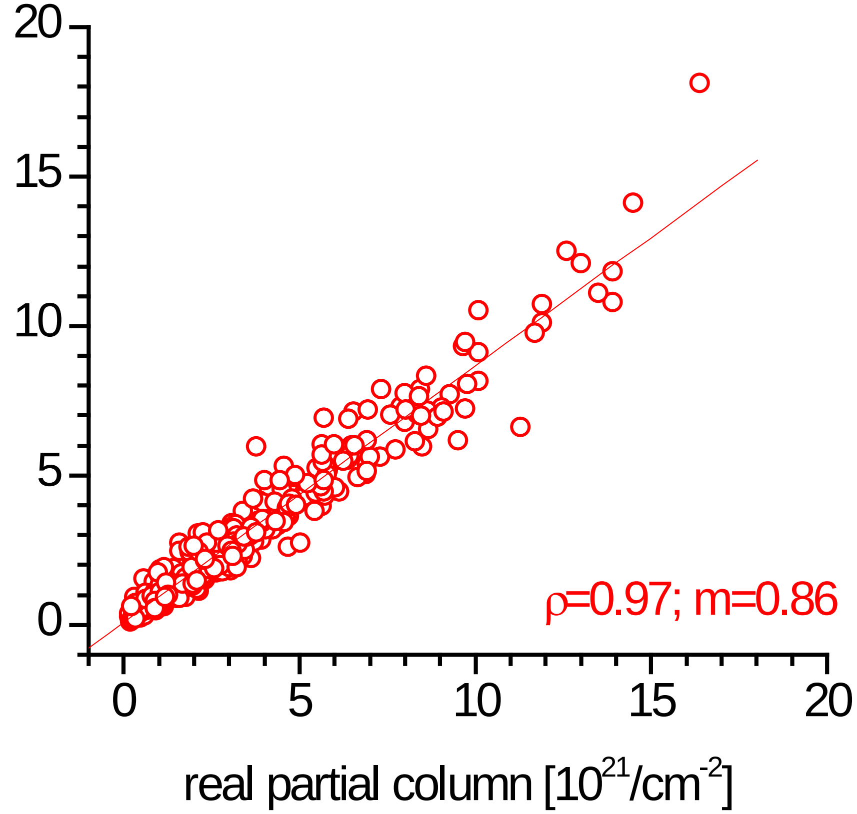


Estimation of total FTIR error (4.3-6.4km):

linear scale



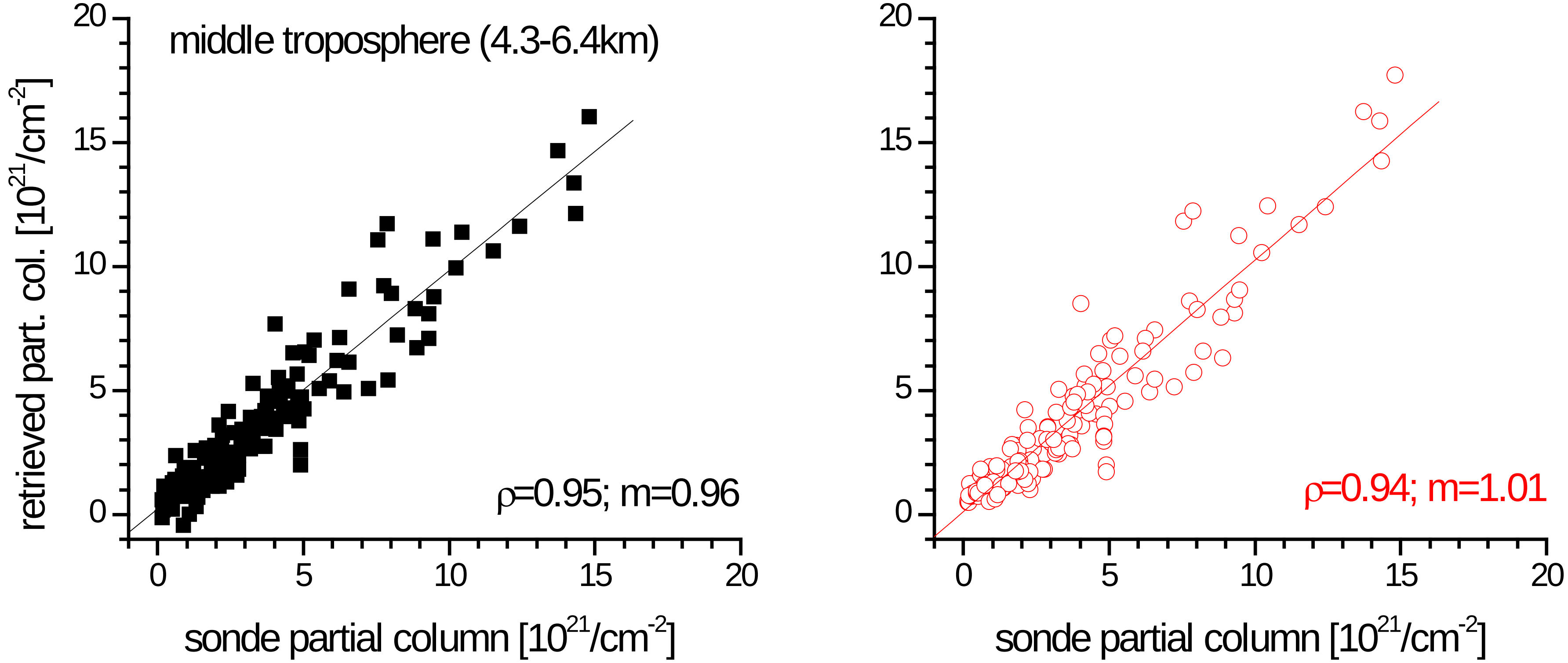
logarithmic scale



FTIR vs. ptu-sonde at 4.3-6.4km:

linear scale

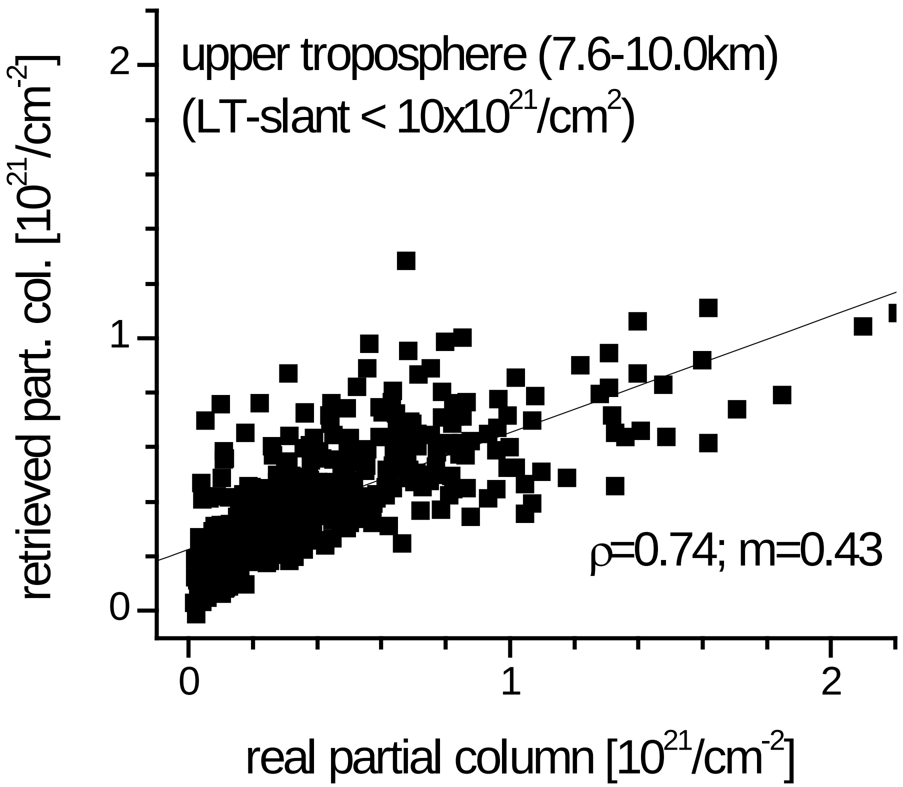
logarithmic scale

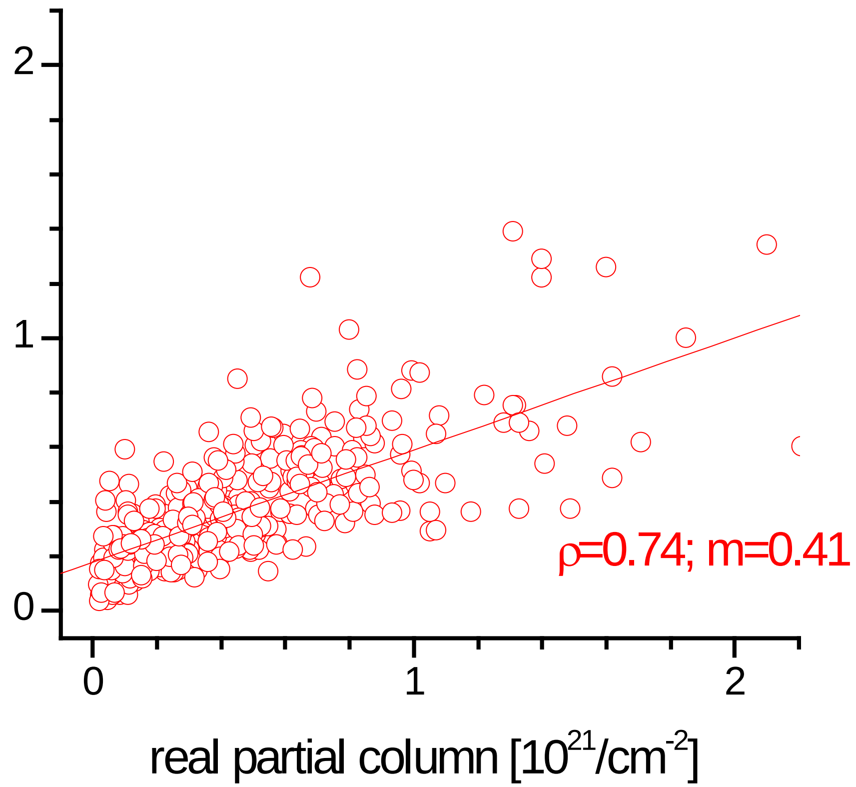


Estimation of total FTIR error (7.6-10.0km):

linear scale

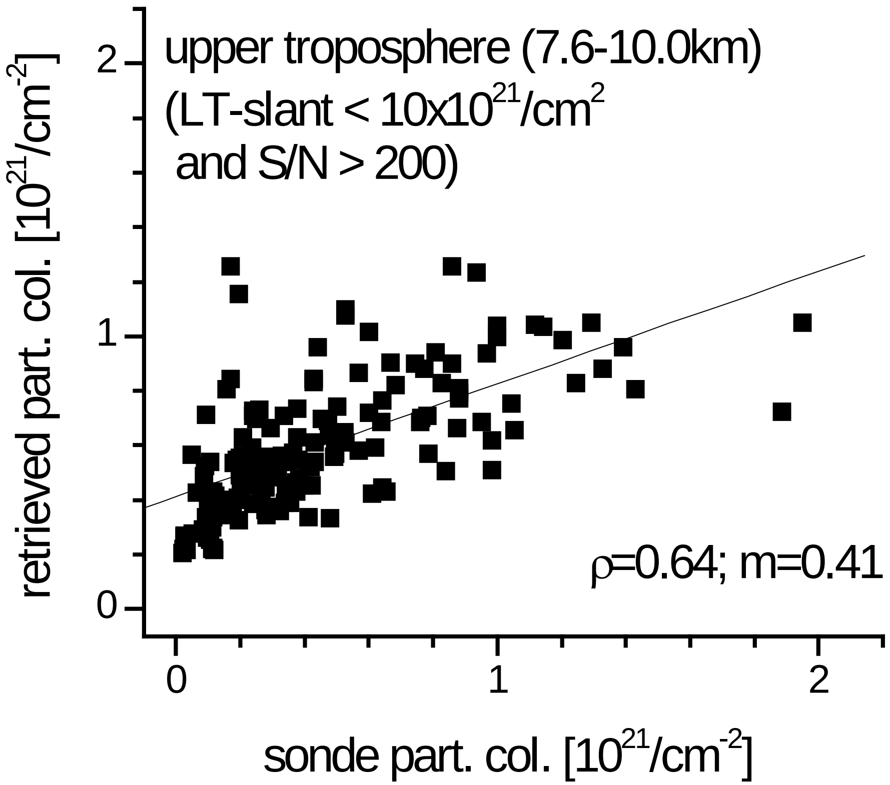
logarithmic scale



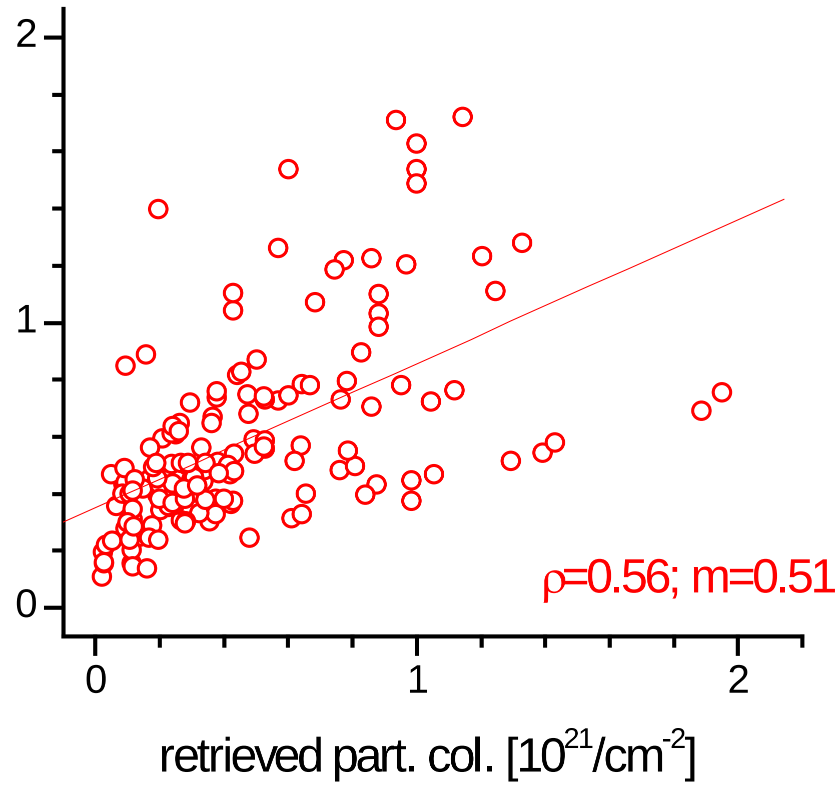


FTIR vs. ptu-sonde at 7.6-10.0km:

linear scale

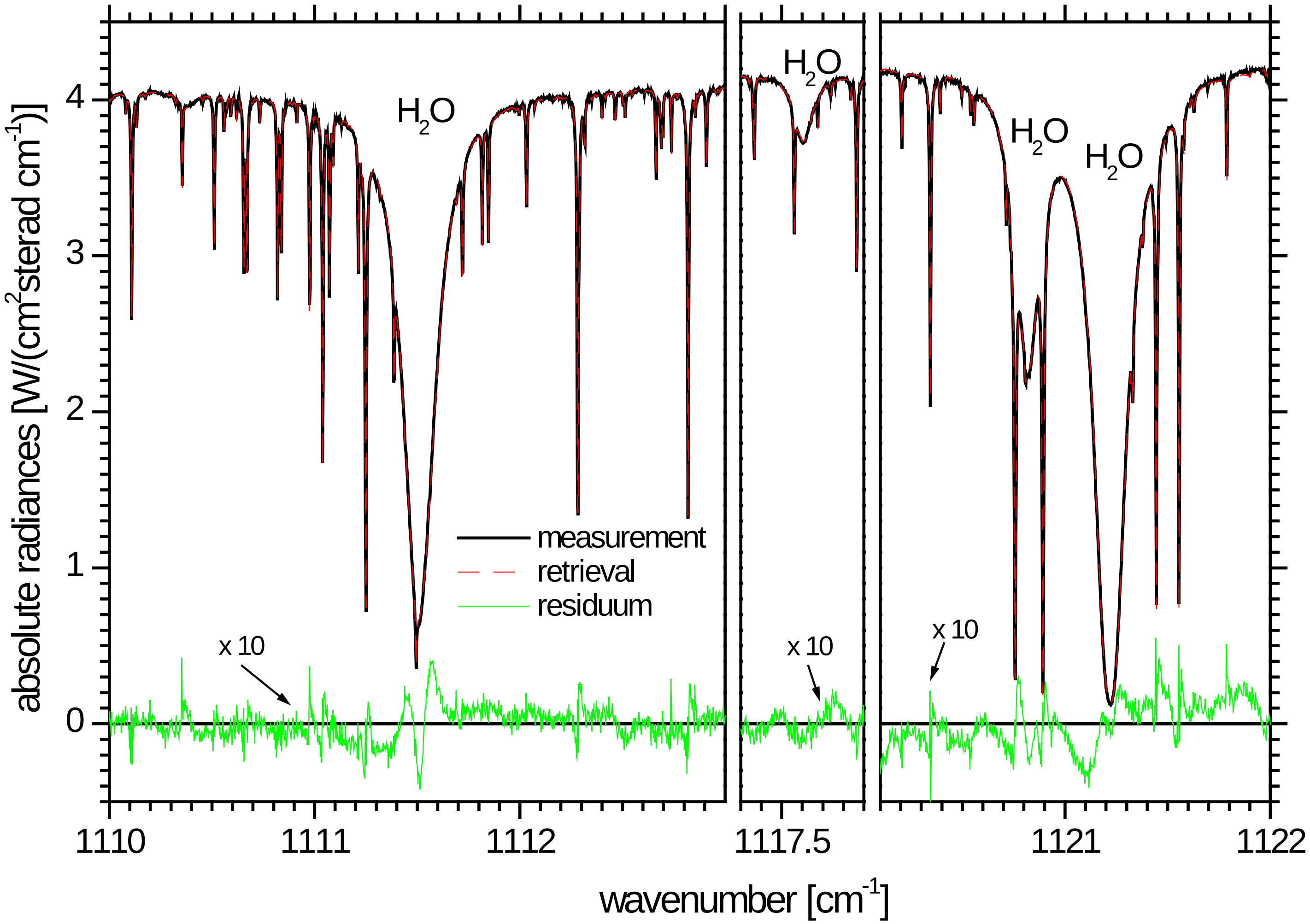


logarithmic scale



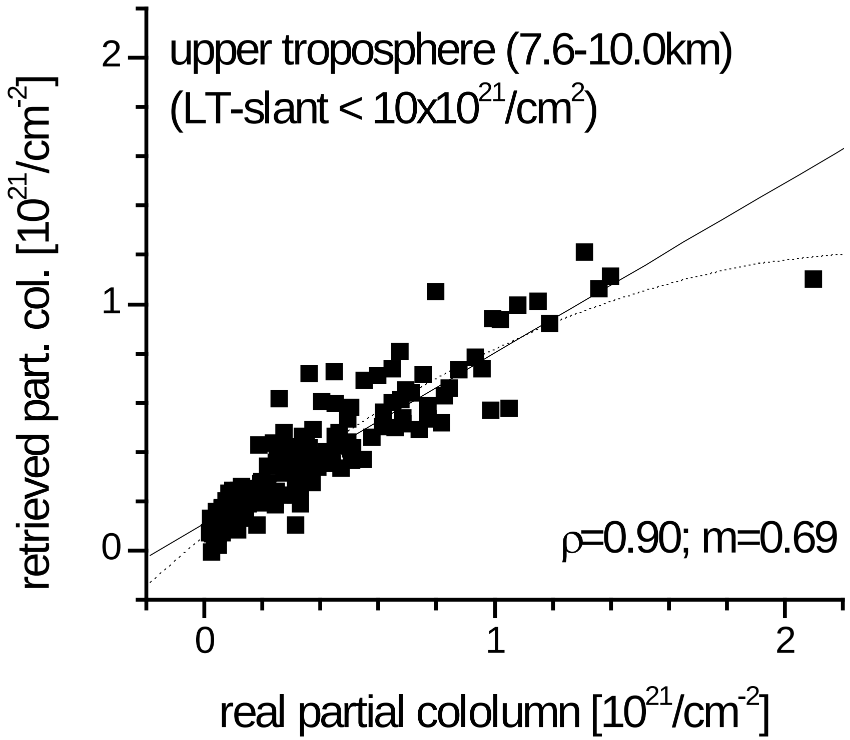
Can we reduce the error of the retrieved UT H_2O amount ?

Case A: Yes, when absorption lines are unsaturated !

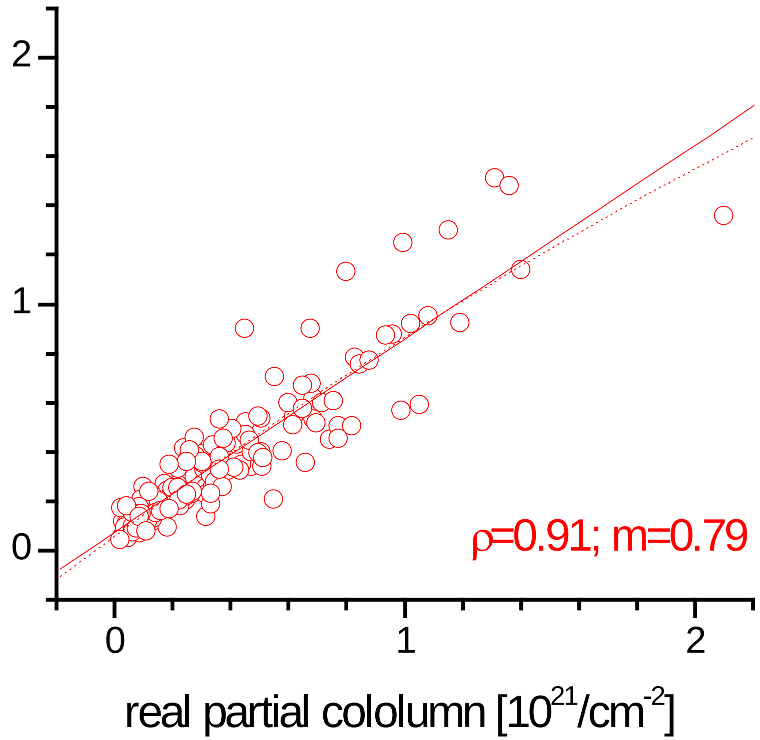


<u>Upper troposphere (Case A)</u>: **Estimation** of total FTIR error for LT slant below 10 x 10^{21}cm^{-2} (7.6-10.0km):

linear scale

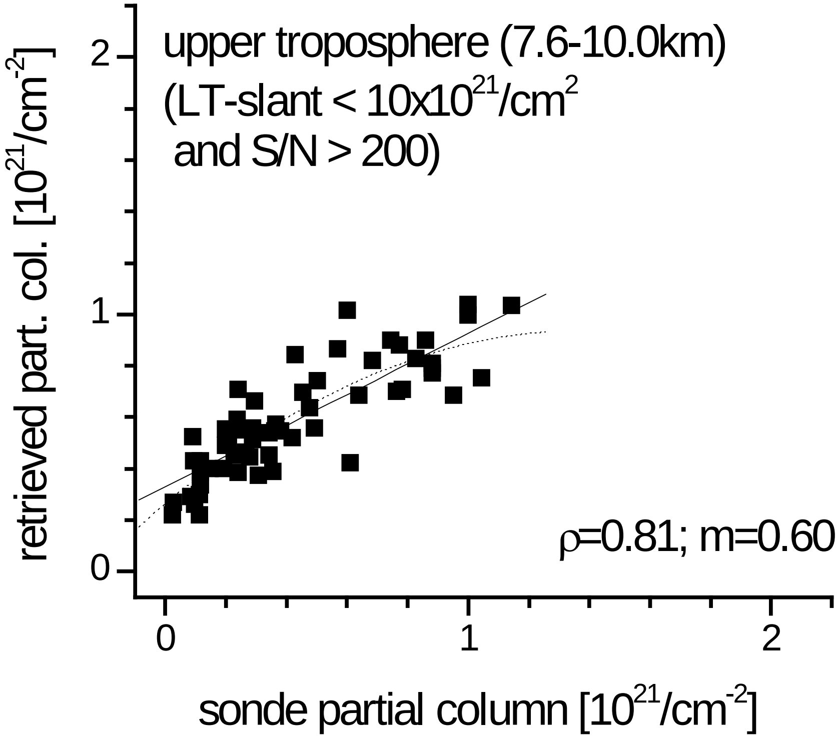


logarithmic scale

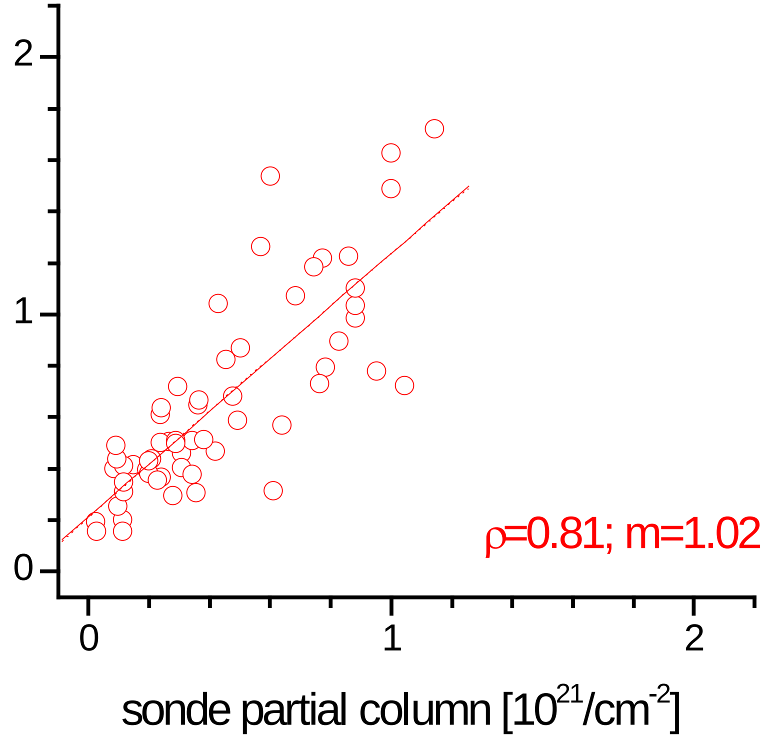


Upper troposphere (Case A): **FTIR vs. ptu-sonde** at 7.6-10.0km for LT slant below 10 x 10^{21}cm^{-1}:

linear scale

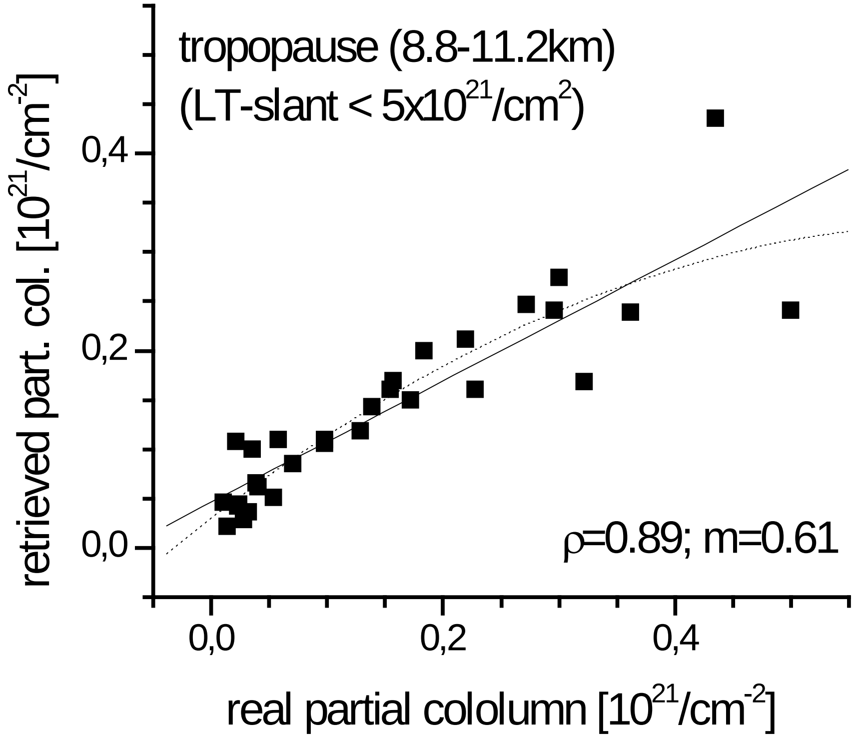


logarithmic scale

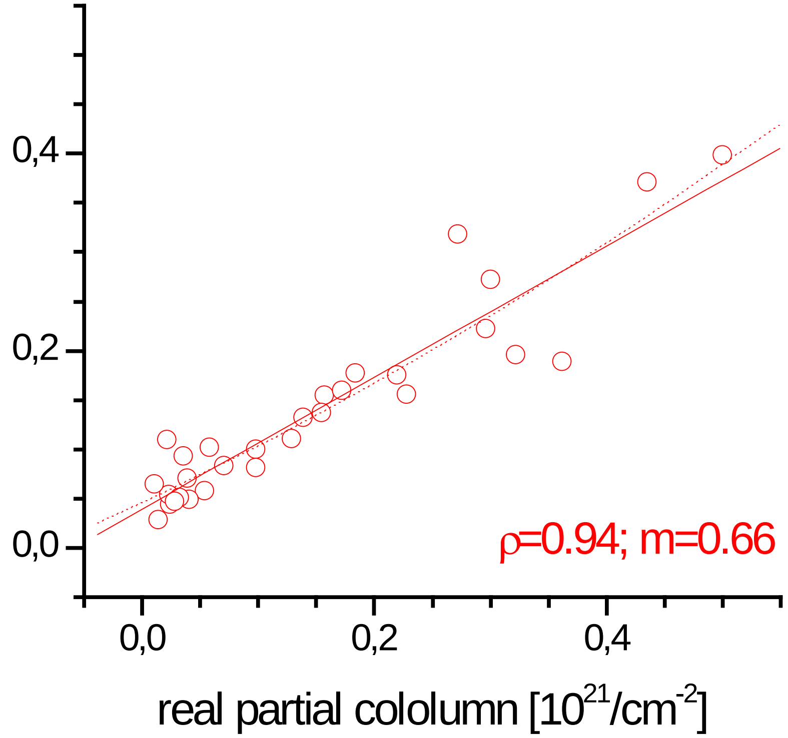


Upper troposphere (Case A): **Estimation** of total FTIR error for LT slant below 5 x 10^{21}cm^{-2} (8.8-11.2km):

linear scale

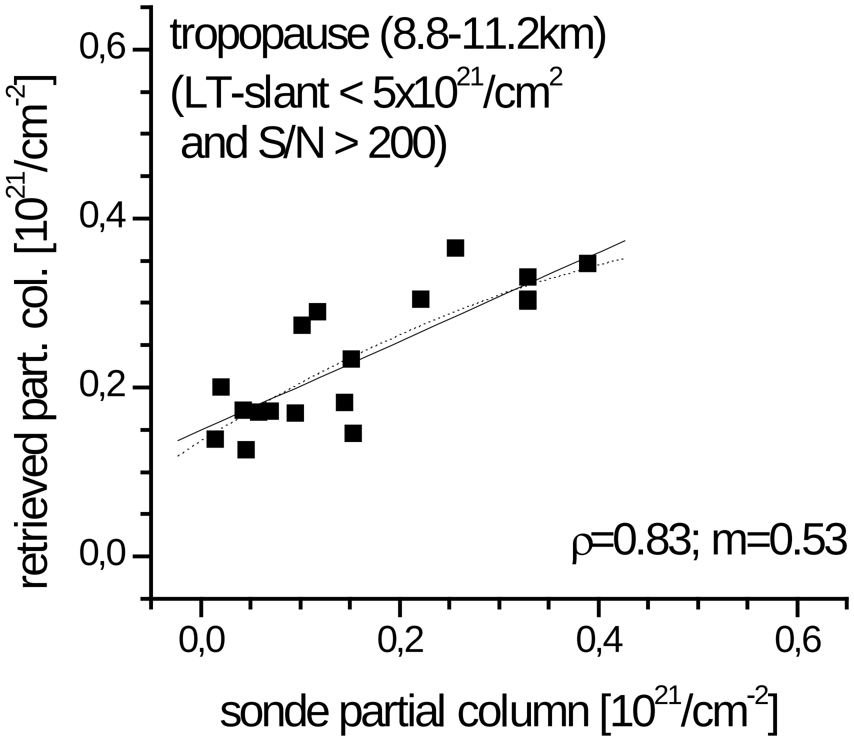


logarithmic scale

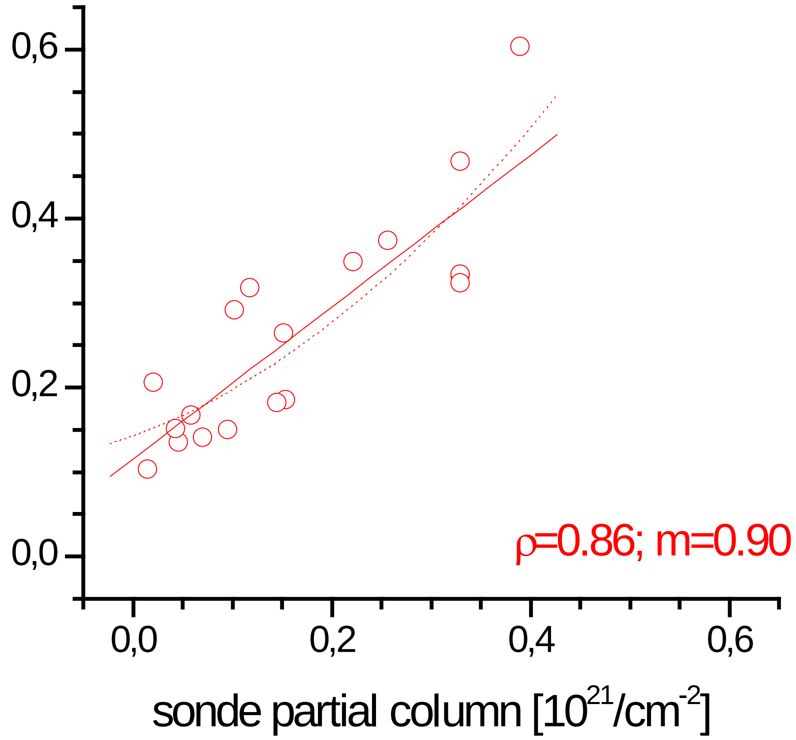


Upper troposphere (Case A): **FTIR vs. ptu-sonde** at 8.8-11.2km for LT slant below 5 x 10^{21}cm^{-1}:

linear scale

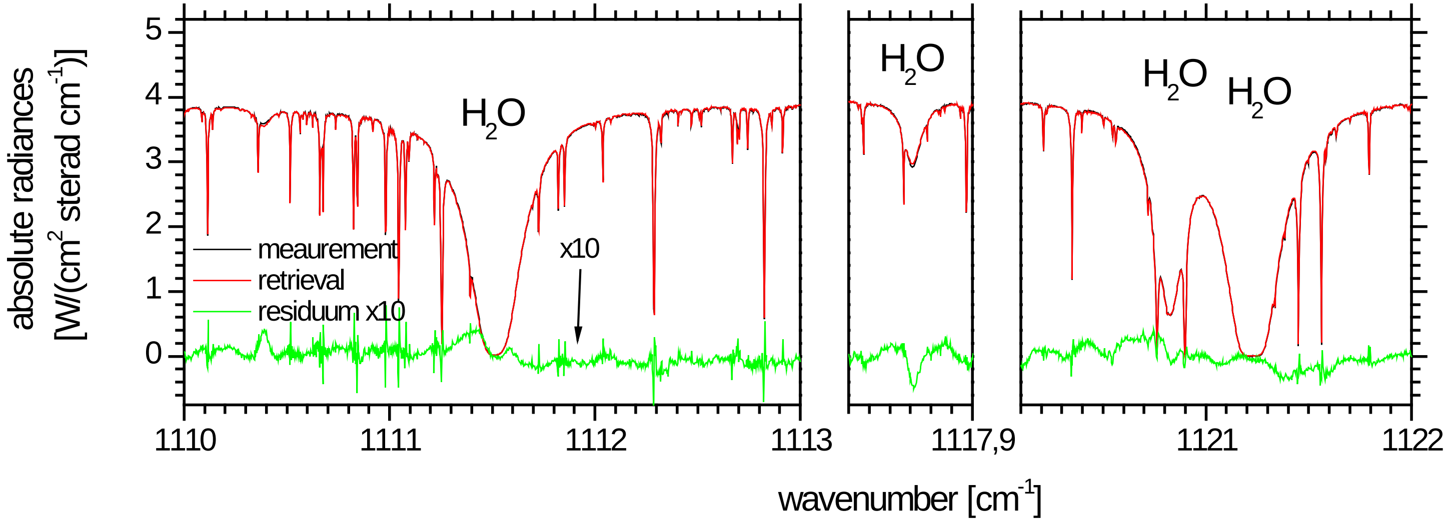


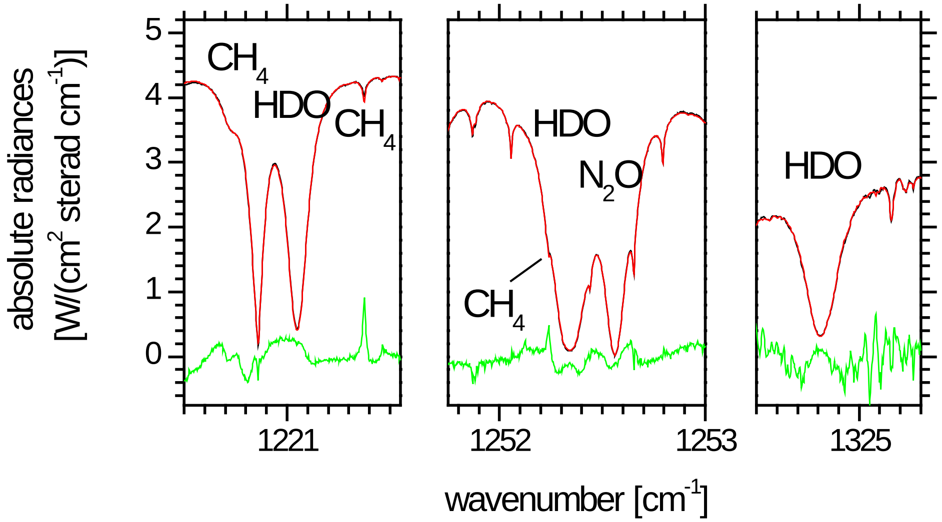
logarithmic scale



Can we reduce the error of the retrieved UT H_2O amount ?

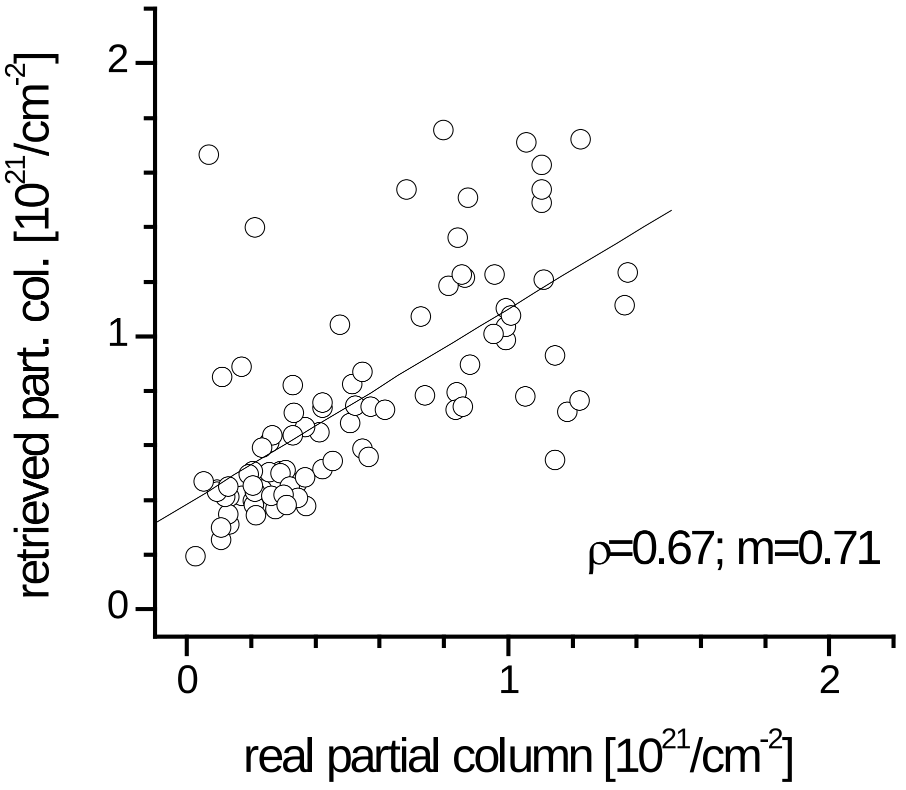
Case B: Yes, when strong and moderately strong lines are fitted simultaneously !



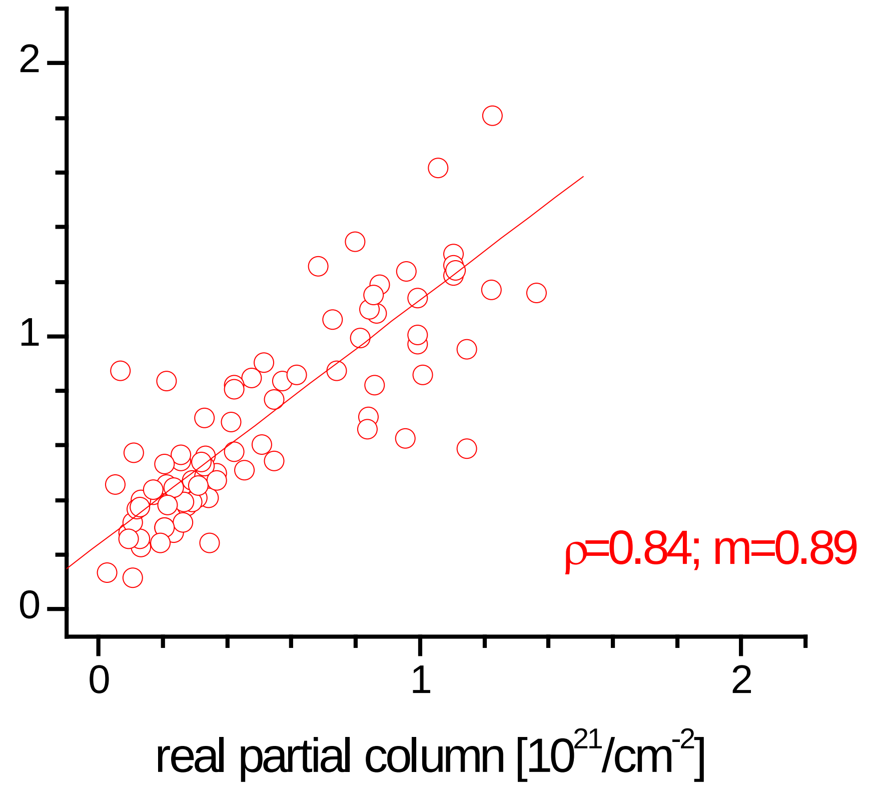


Upper troposphere (Case B): **FTIR vs. ptu-sonde** at 7.6-10.0km (LT slant below 25 x $10^{21}cm^{-2}$):

strong lines

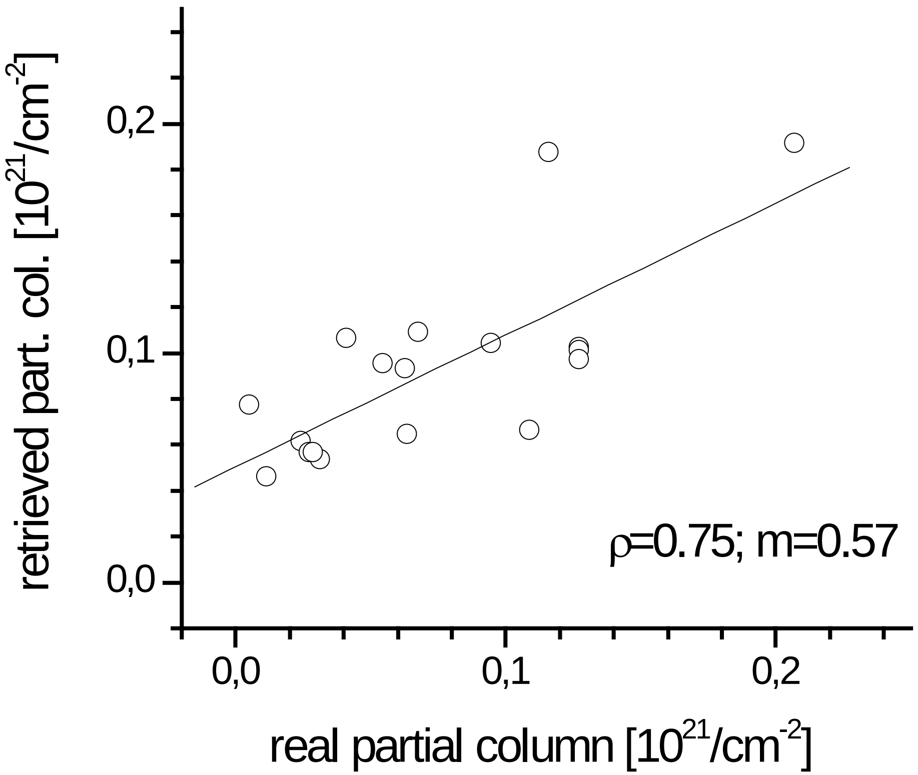


strong and moderately strong lines

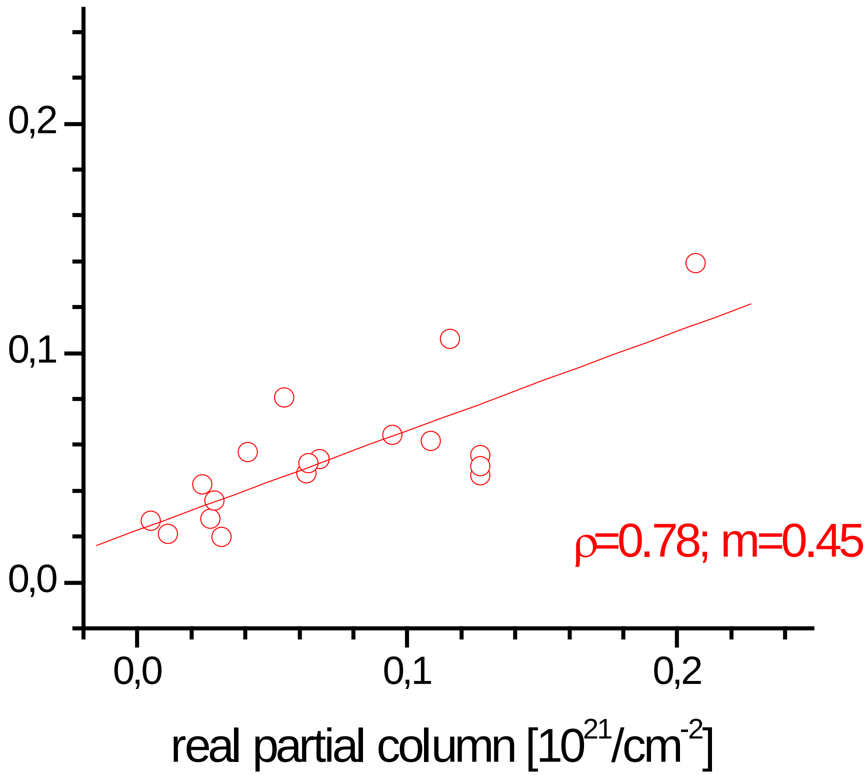


Upper troposphere (Case B): **FTIR vs. ptu-sonde** at 10.0-12.4km (LT slant below 5 x 10^{21}cm^{-2}):

strong lines



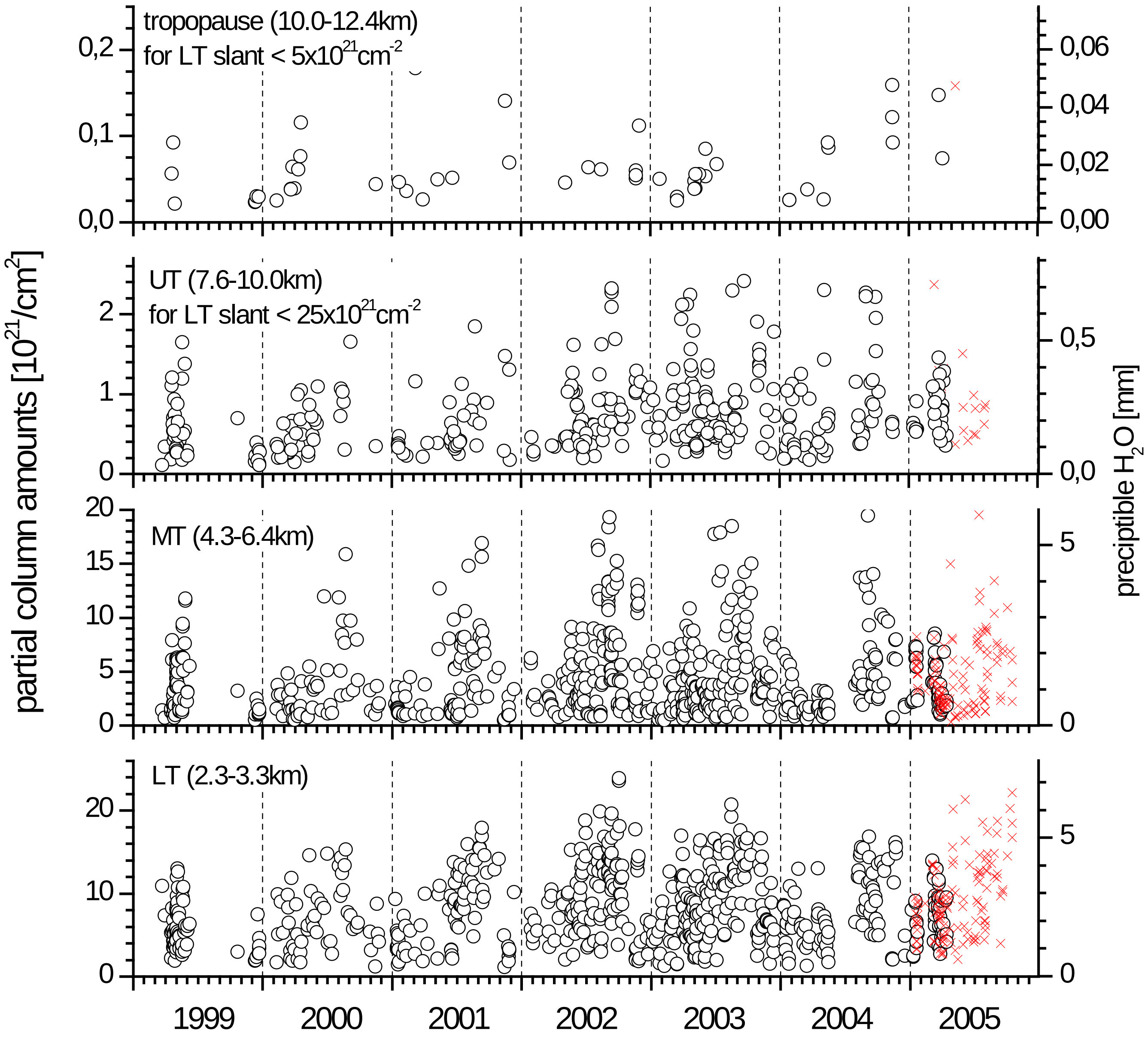
strong and moderately strong lines



Recipe for retrieval of upper tropospheric H_2O:

- Only retrieval on a logarithmic scale provides for a correctly posted cost function → this reduces the systematic errors if compared to a retrieval on linear scale. It leads to consistent time series and a good sensitivity for UT H_2O amounts
- Simultaneous fit of strong and moderately strong lines provides for best exploitation of spectra → makes continuous observation of UT H2O feasible
- Most important errors are: smoothing error, ILS, line parameter, and temperature profile

3. 7-year record of water vapour above Izaña observatory



Above 9km retrieval requires unsaturated H_2O lines → LT slant below 5 x 10^{21} cm^{-2} (in Izaña only for 10% of all measurements)

Above 7.5km retrieval requires moderate LT H_2O amounts and simultaneous fit of strong and moderately strong lines

Up to 7km retrieval possible under all measurement conditions

Our study shows the following:

1. FTIR well-suited for continuous monitoring of lower and middle tropospheric H_2O amounts.

2. For upper tropospheric H_2O amounts a continuous monitoring is tricky, but feasible by FTIR, if:
   A: the inversion is perform on a log-scale
   B: strong and moderately strong lines are fitted simultaneously

Future work:

1. Produce continuous time series of UT water vapour from many historic FTIR measurements (e.g. measurements at Jungfraujoch or Kitt Peak could produce unique continuous 20-year records !)

2. Further improvements are still possible for dryer or higher situated sites:
   we could apply stronger H_2O lines → improved sensitivity at higher altitudes. Detection of lower stratospheric water vapour variability from Jungfraujoch ?

3. Retrieval of HDO/H_2O

Thank You !!!!!!!!!

Summary of differences between FTIR and ptu sonde data (sum of errors of sonde and FTIR). Theoretical estimations of FTIR errors are in brackets:

linear scale:

	total	2.3-3.3km	4.3-6.4km	7.6-10.0km	8.8-11.2km
random	**25 (4)**	**40 (21)**	**32 (24)**	**54 (50)**	**56 (47)**
systematic[(A)]	**+6 (0)**	**+3 (-3)**	**-4 (-6)**	**-40 (-31)**	**-47 (-38)**

logarithmic scale:

	total	2.3-3.3km	4.3-6.4km	7.6-10.0km	8.8-11.2km
random	**25 (4)**	**47 (22)**	**33 (24)**	**58 (49)**	**51 (42)**
sytematic[(A)]	**+6 (-1)**	**-4 (-4)**	**+1 (-1)**	**+2 (-23)**	**-10 (-33)**

(A): systematic spectroscopic line parameter errors are not considered

Upper troposphere (Case B): **Estimation** of total FTIR error at 7.6-10.0km (LT slant below 25 x $10^{21}cm^{-2}$):

strong lines

strong and moderately strong lines

Upper troposphere (Case B): **Estimation** of total FTIR error at 7.6-10.0km (LT slant below 25 x $10^{21}cm^{-1}$):

strong lines

strong and moderately strong lines

What about the averaging kernels ?

In the case of water vapour the averaging kernels only contain limited information about the sensitivity of the measurements.

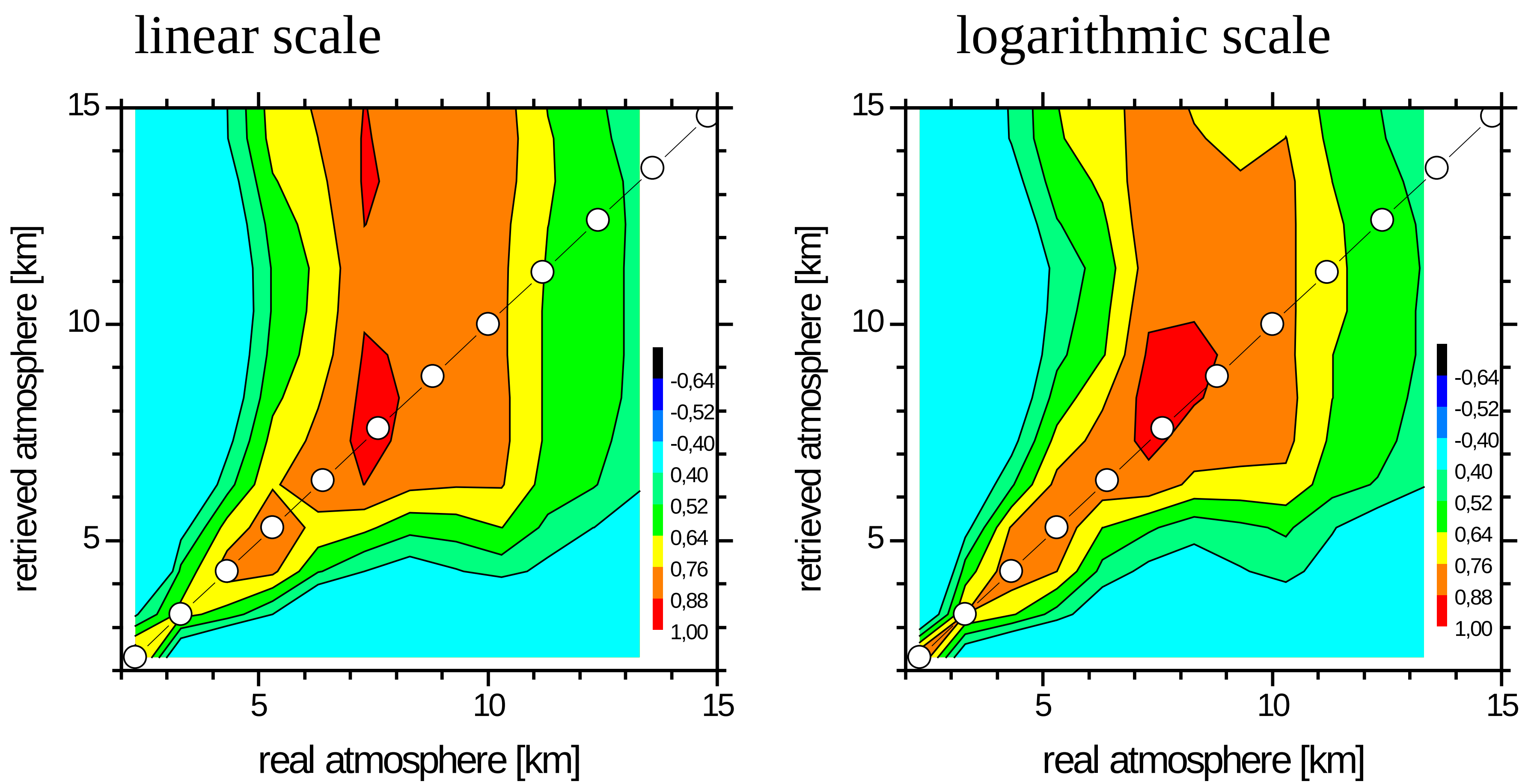
Reason:

1. Non-linearities (kernels depend strongly on actual H_2O profile)
2. variability of H_2O decreases with height by 4 orders of magnitude
   → comparison of kernels for different heights is not straight forward !

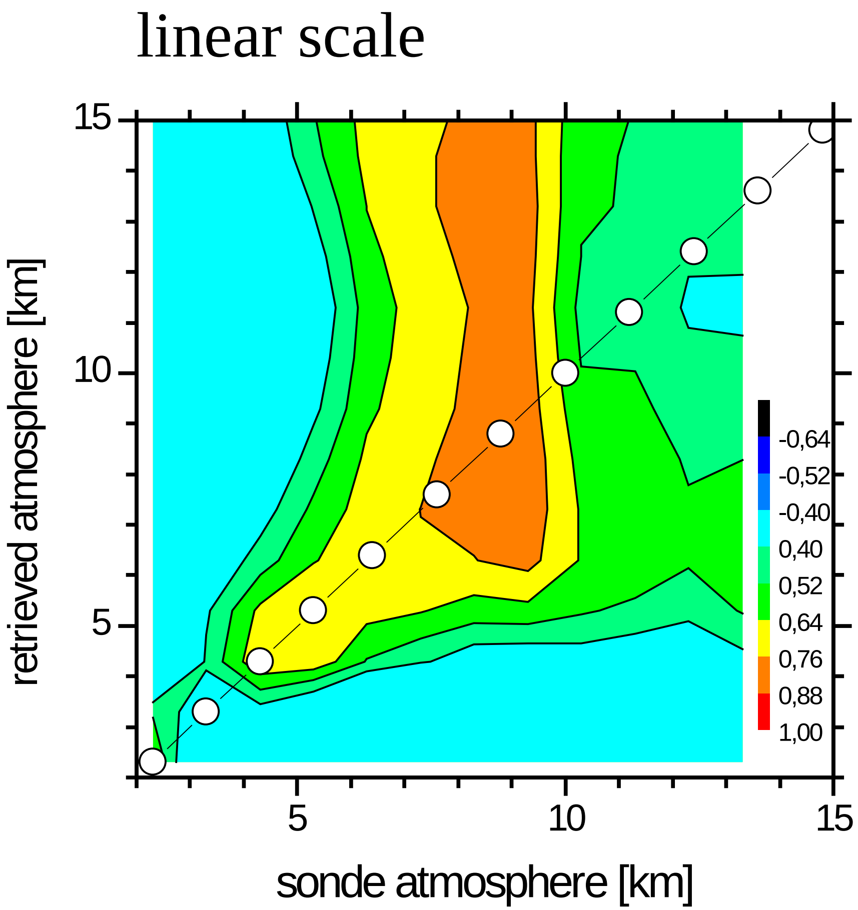
Alternative representation of sensitivity:

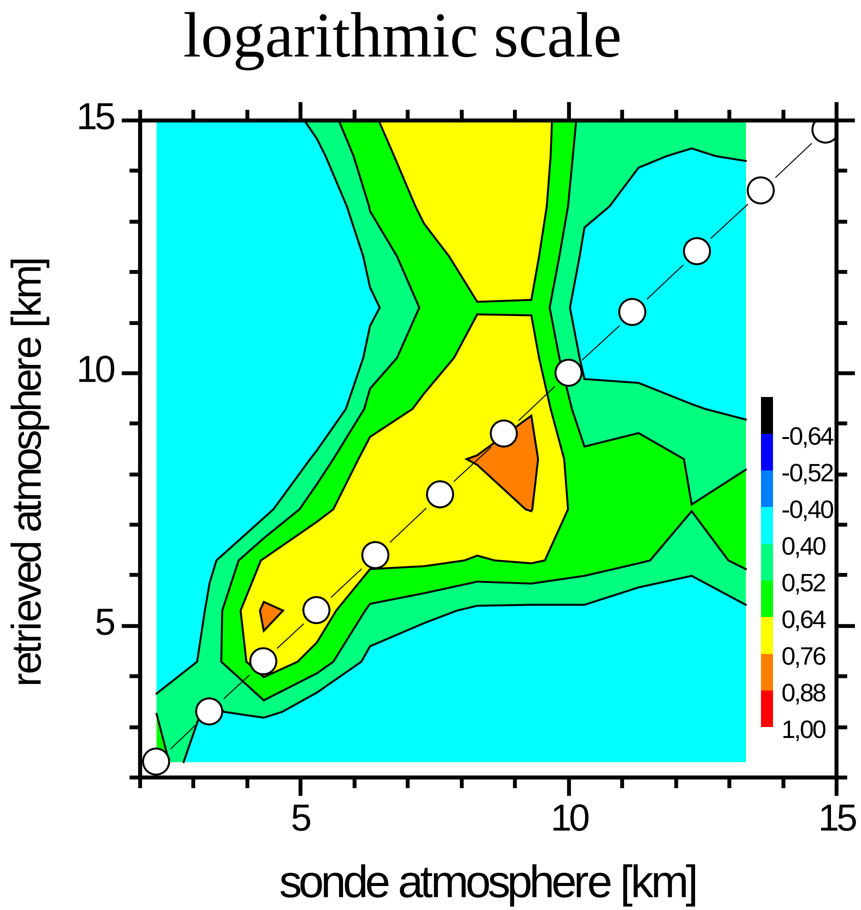
Correlation matrices (correlation between original profiles and inverted profiles). The matrices give a realistic overview of the detectable atmospheric regions. Furthermore, they allow us to perform this sensitivity analysis for a realistic error scenario.

Estimation for LT slant column below 10 x 10^{21}cm^{-2}:



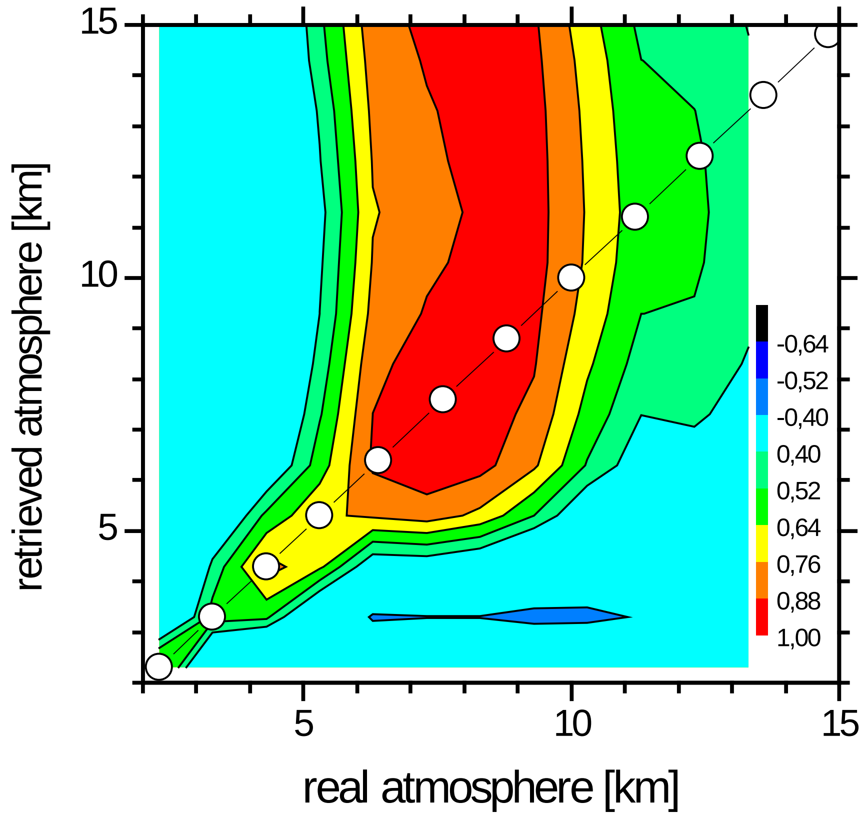
FTIR vs. sonde for LT slant below 10 x 10^{21}cm^{-2}:



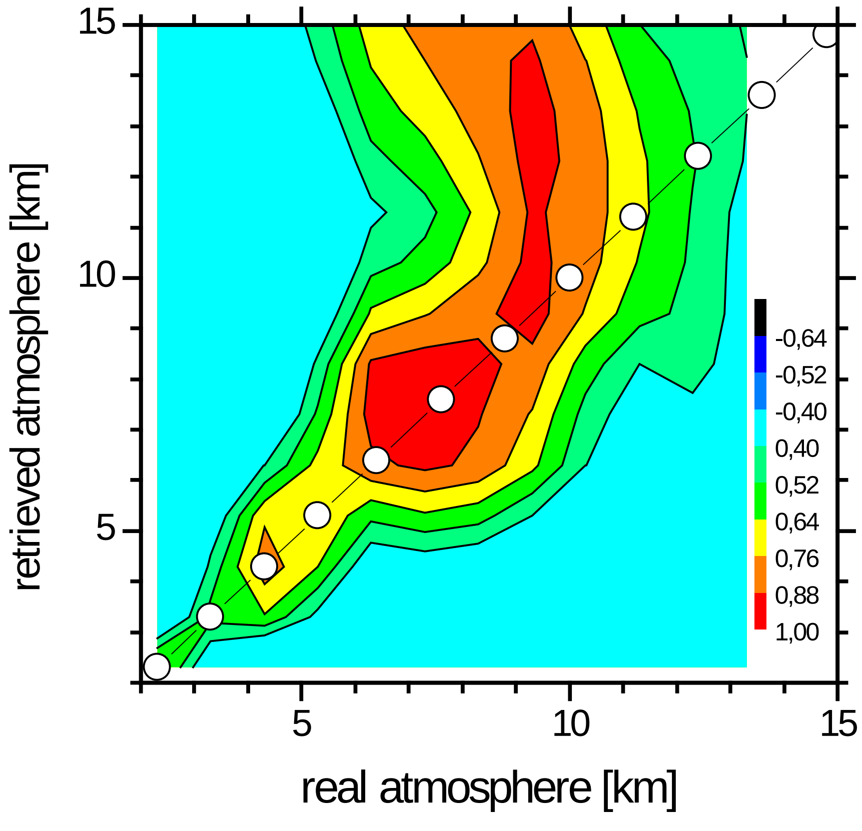


Estimation for LT slant column below 5 x 10^{21}cm^{-2}:

linear scale



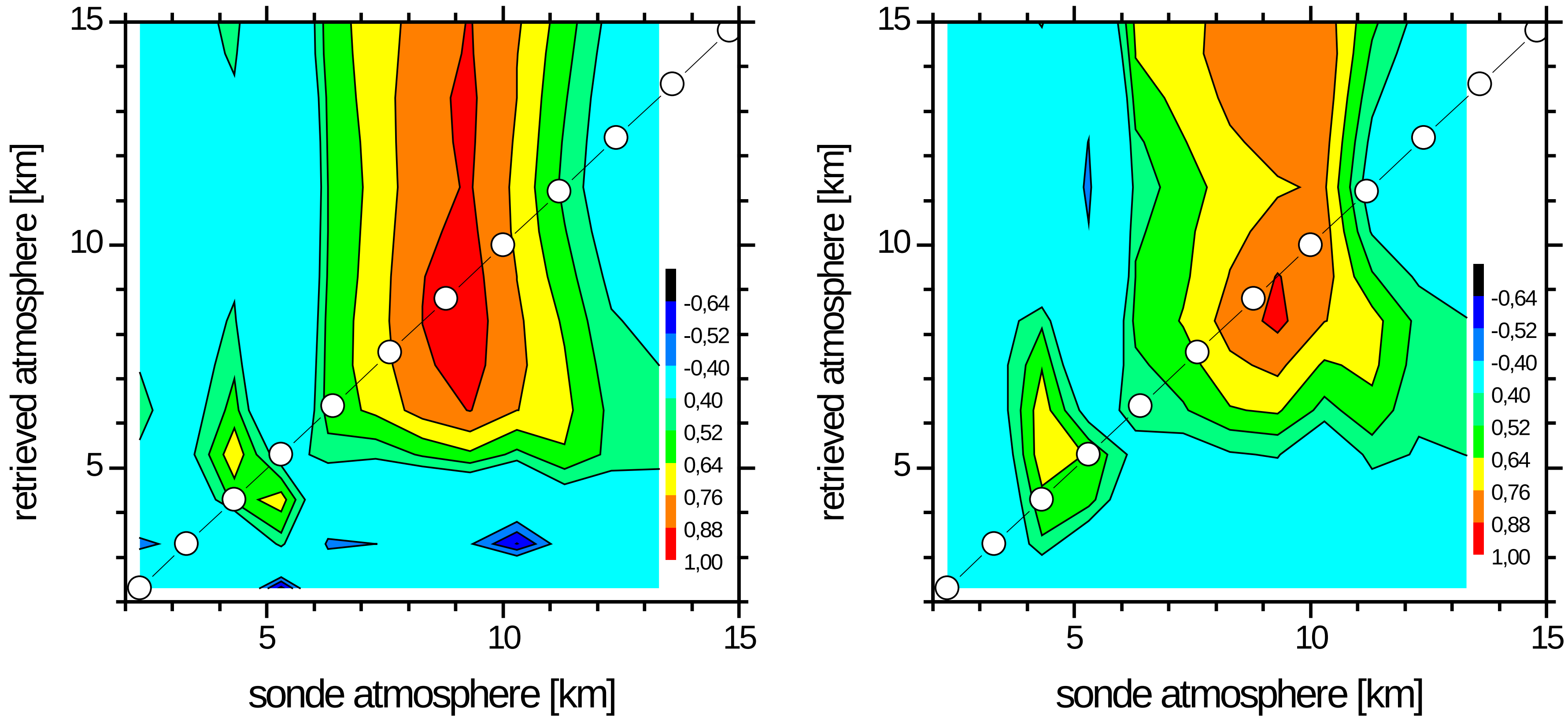
logarithmic scale



FTIR vs. sonde profiles for LT slant < 5 x 10^{21} cm^{-2}:

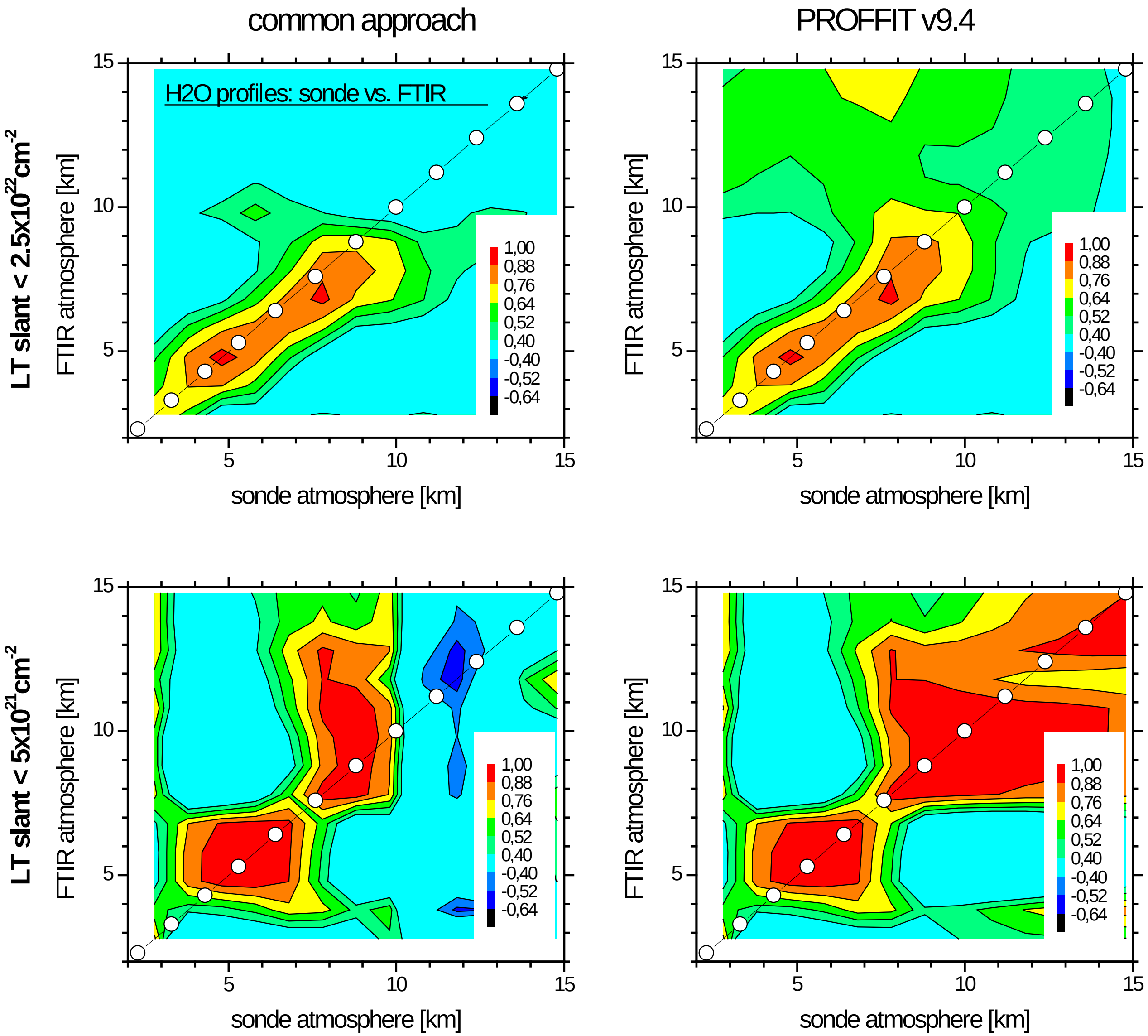
linear scale

logarithmic scale



Slide from talk “Ground-based remote sensing of tropospheric HDO/H2O ratio profiles”

Empirical validation of H_2O profiles: ptu-sonde vs. FTIR:



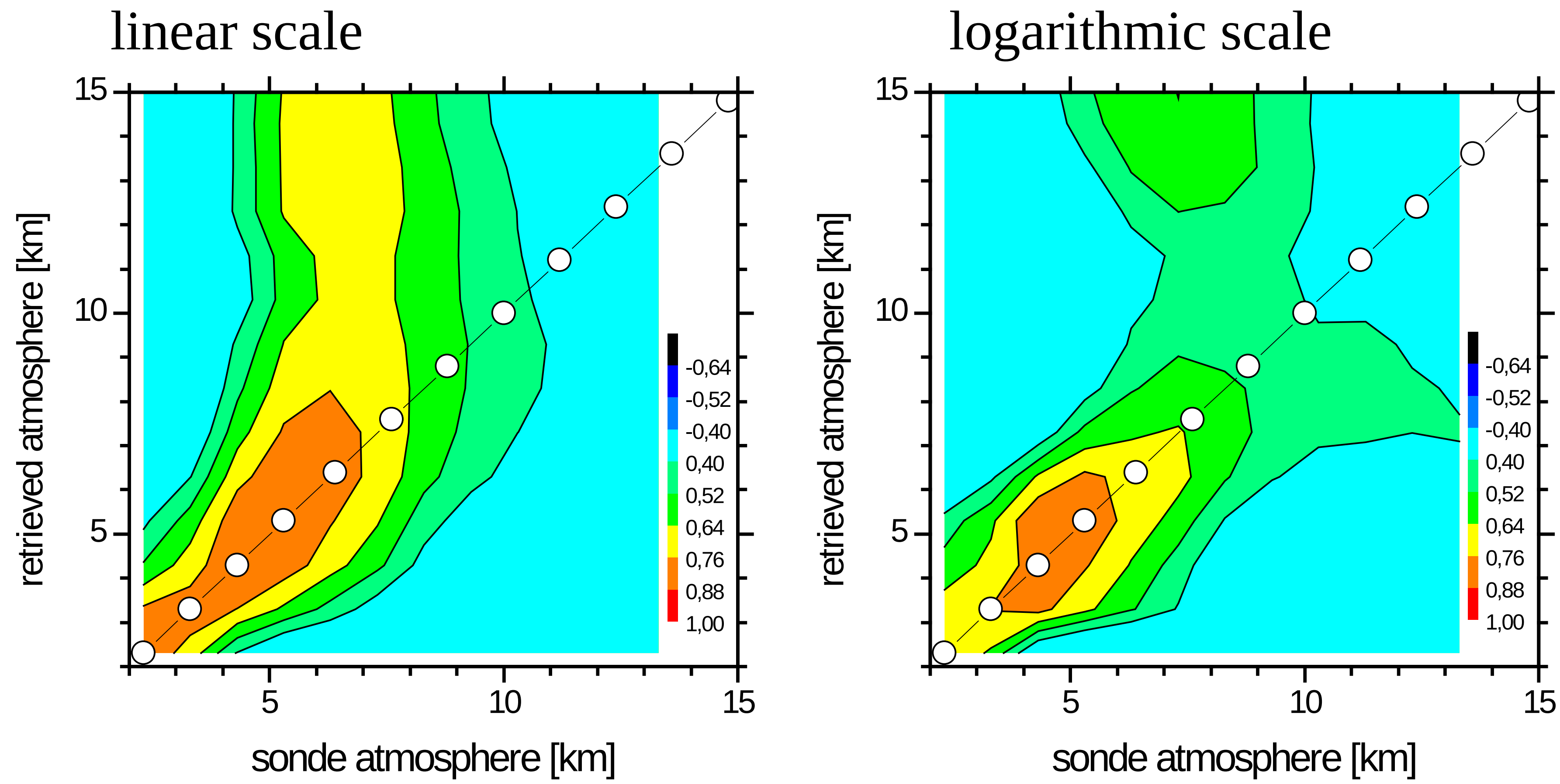
Inter-species constraint not only improves quality of δD profiles but also quality of H_2O profile:

H_2O retrieval benefits from additional information present in HDO lines

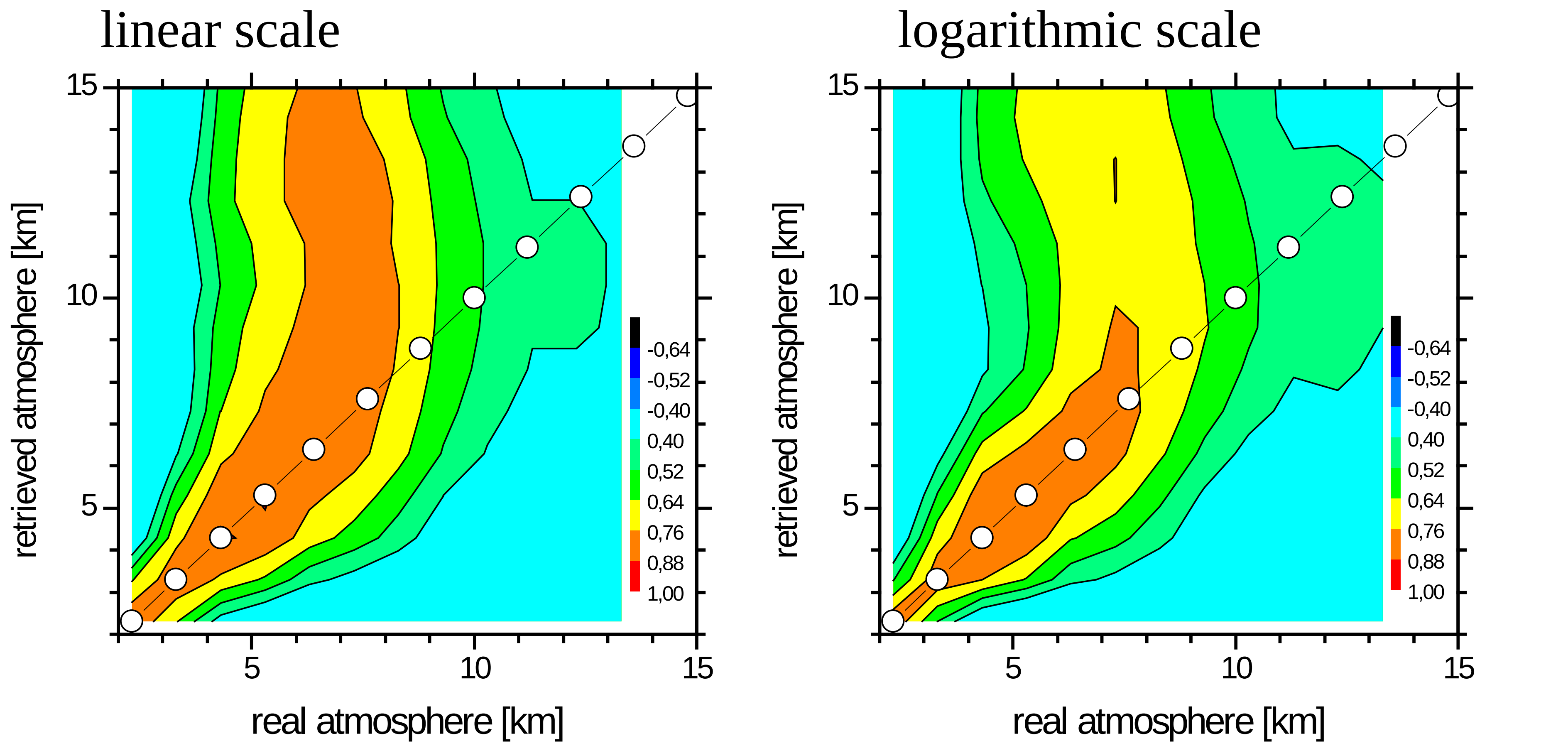
Detection of UT/LS H_2O with the proposed lines ?

For a definitive conclusion we need a larger ensemble of compared profiles (the correlation shown here bases on only 7 profiles) !

FTIR versus sonde profiles for all measurement days:

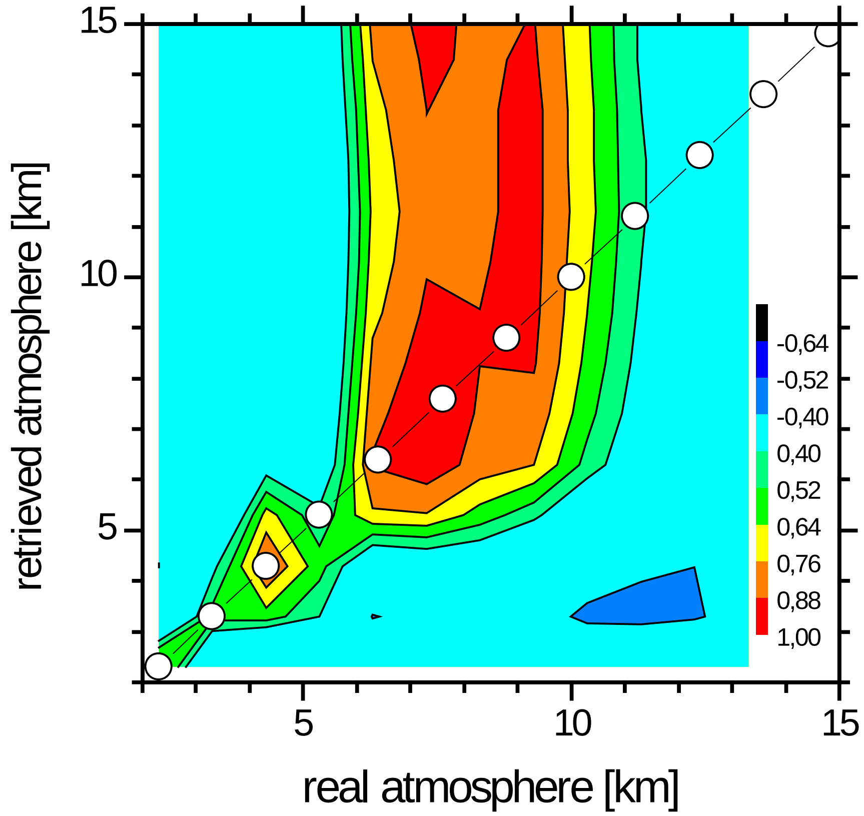


Corresponding theoretical sensitivity assessment (whole ensemble):

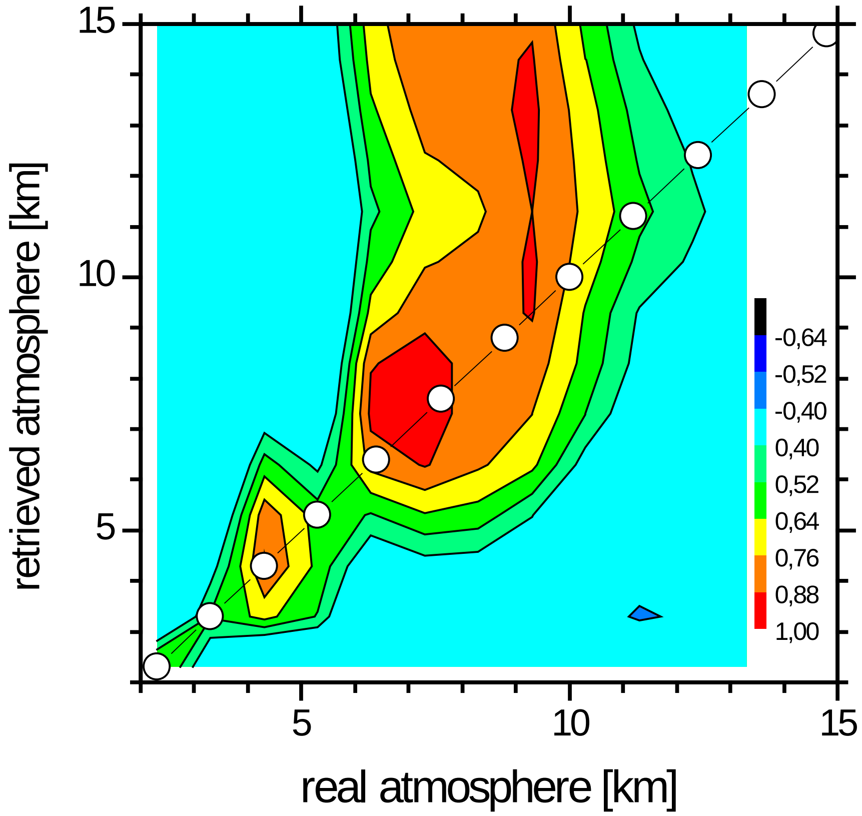


Corresponding theoretical sensitivity assessment (LT slant < 5 x 10^{21}cm^{-2}):

linear scale



logarithmic scale



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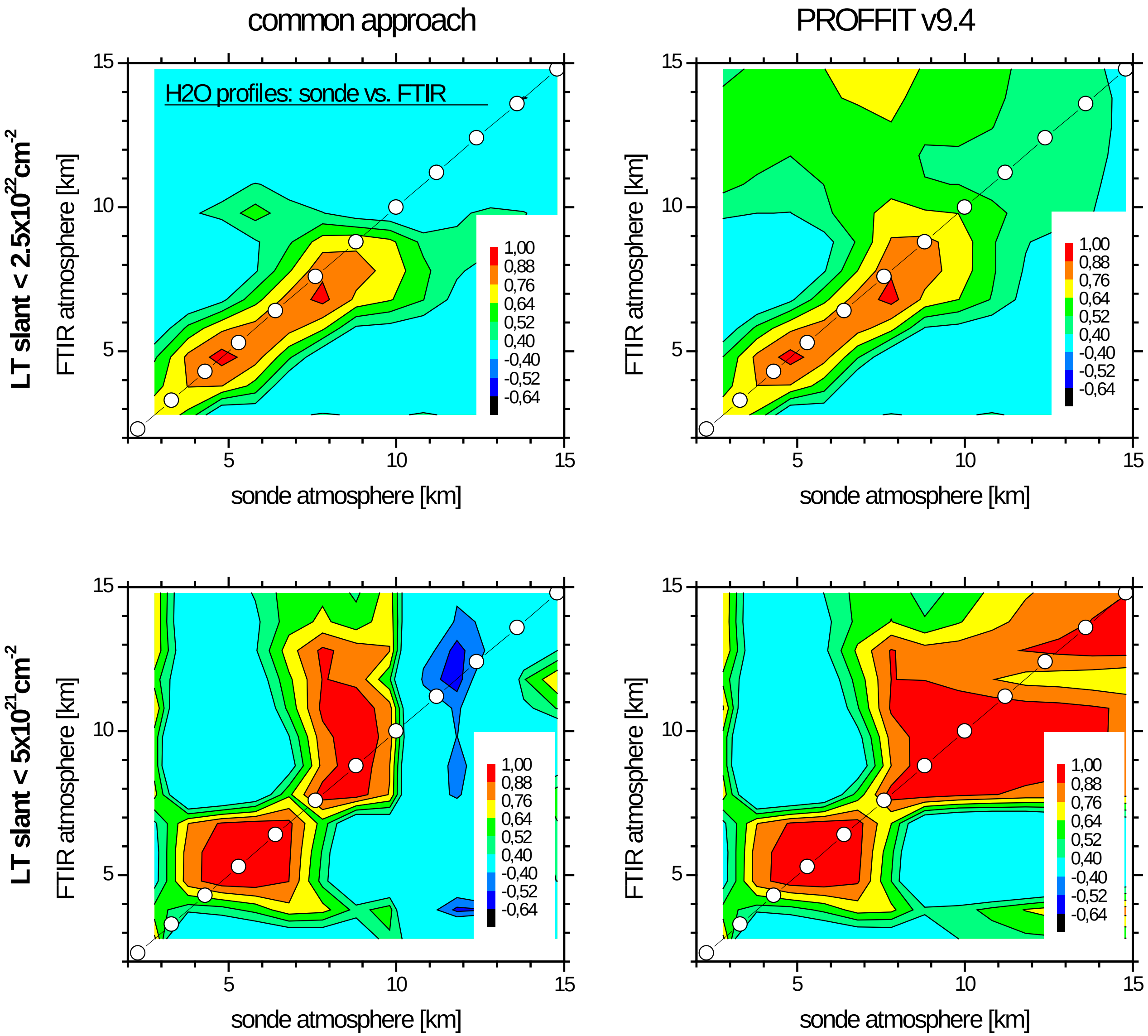

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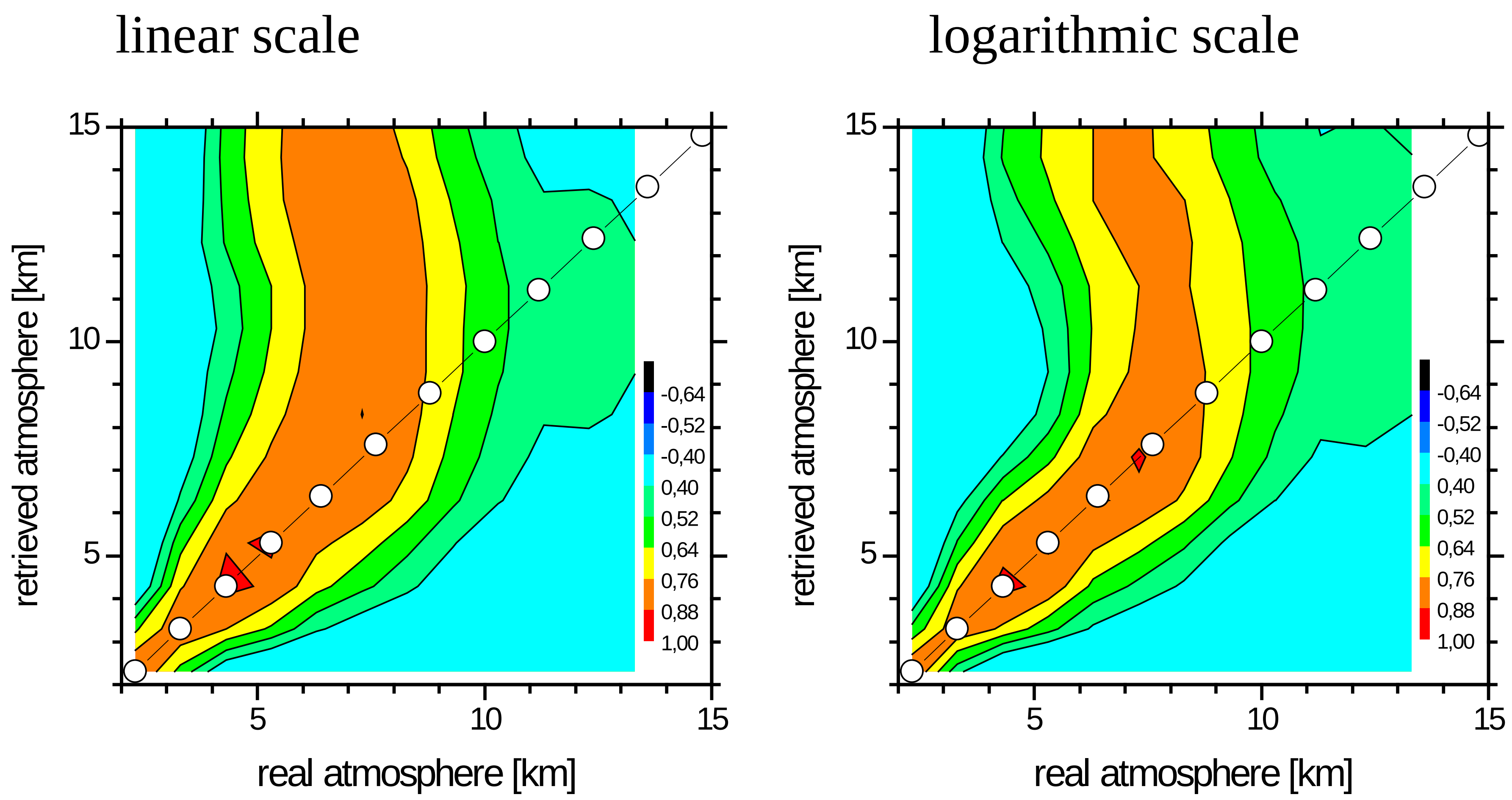
Whole ensemble:



Error estimation by means of linear least squares fit

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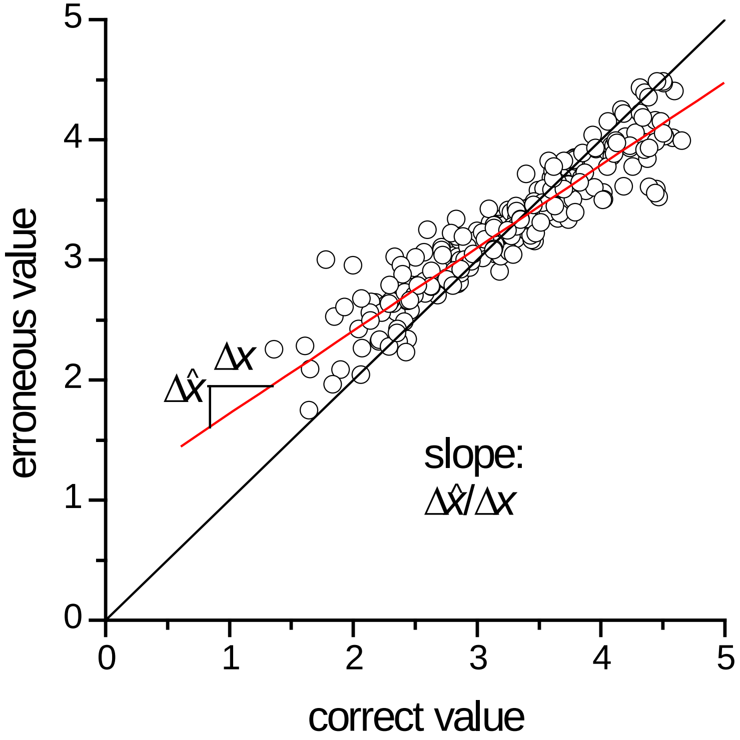
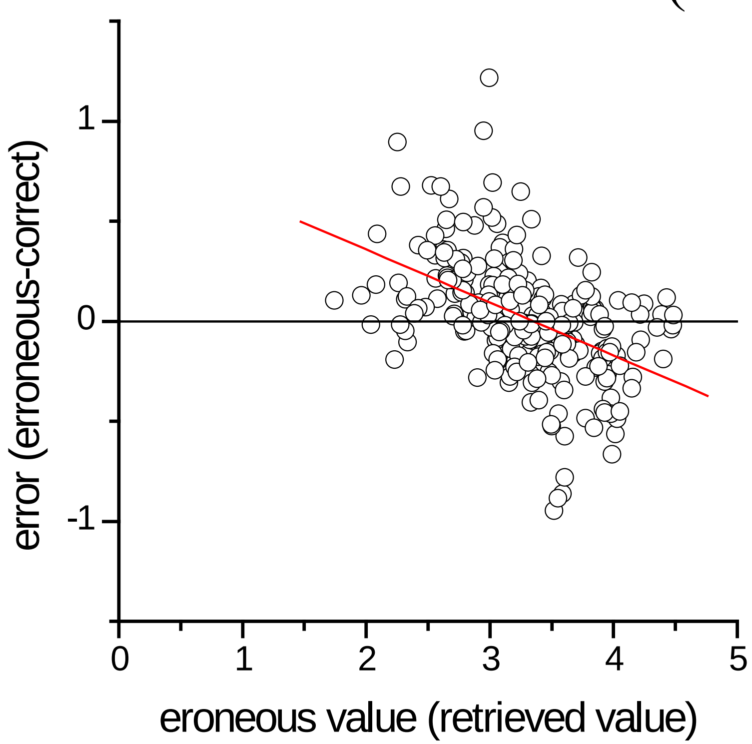
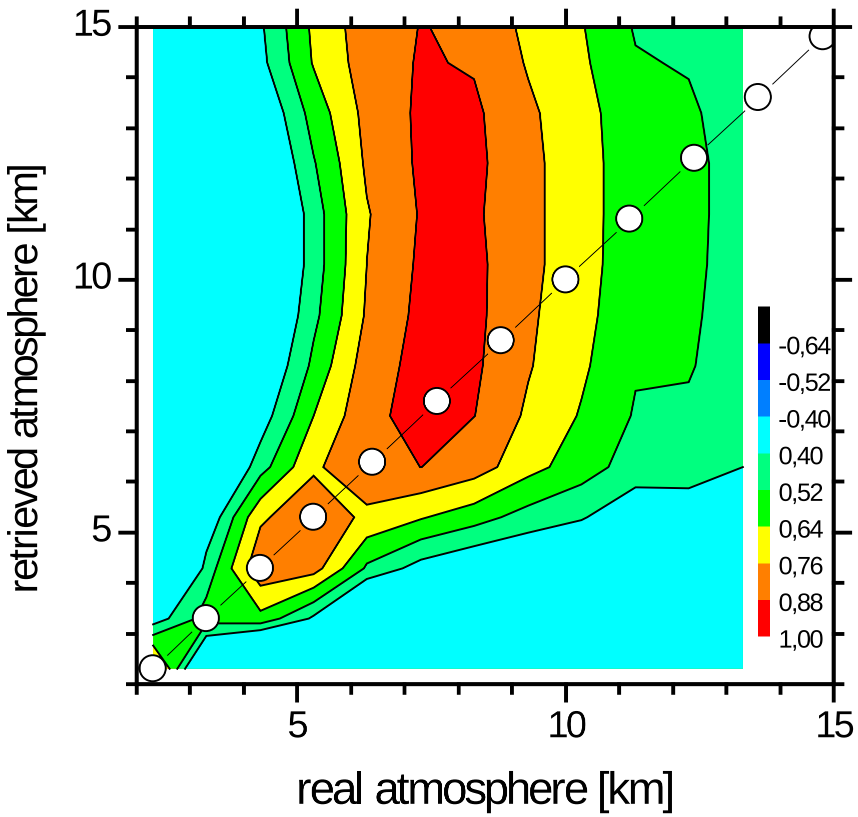


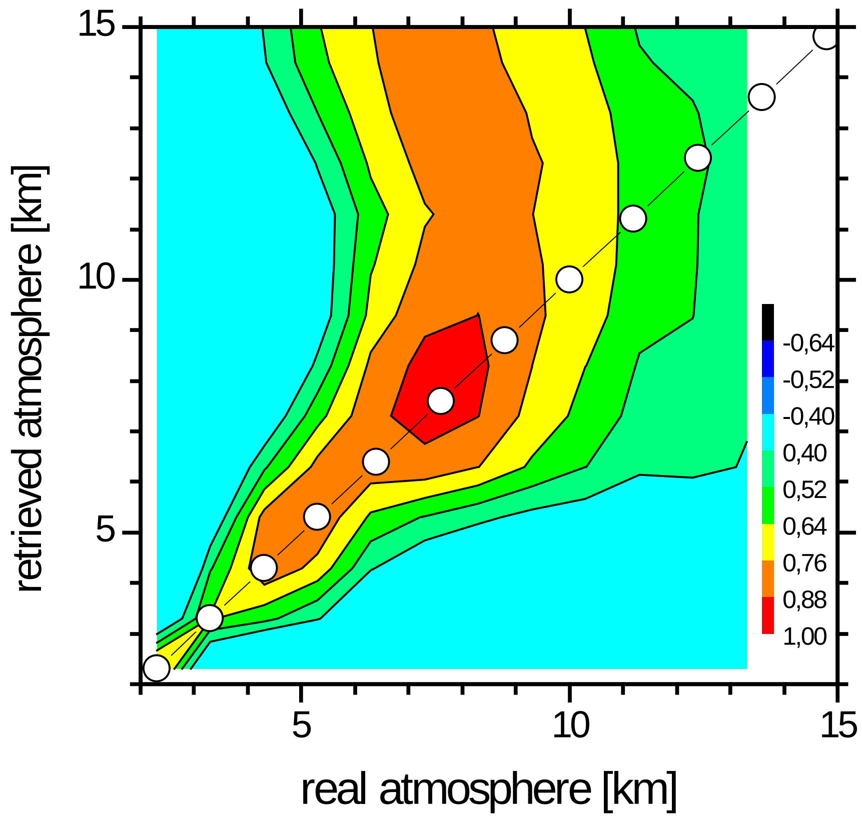


Slant column of lower troposphere (2.3-4.3km) below 10 x 10^{21}cm^{-2}:

linear scale

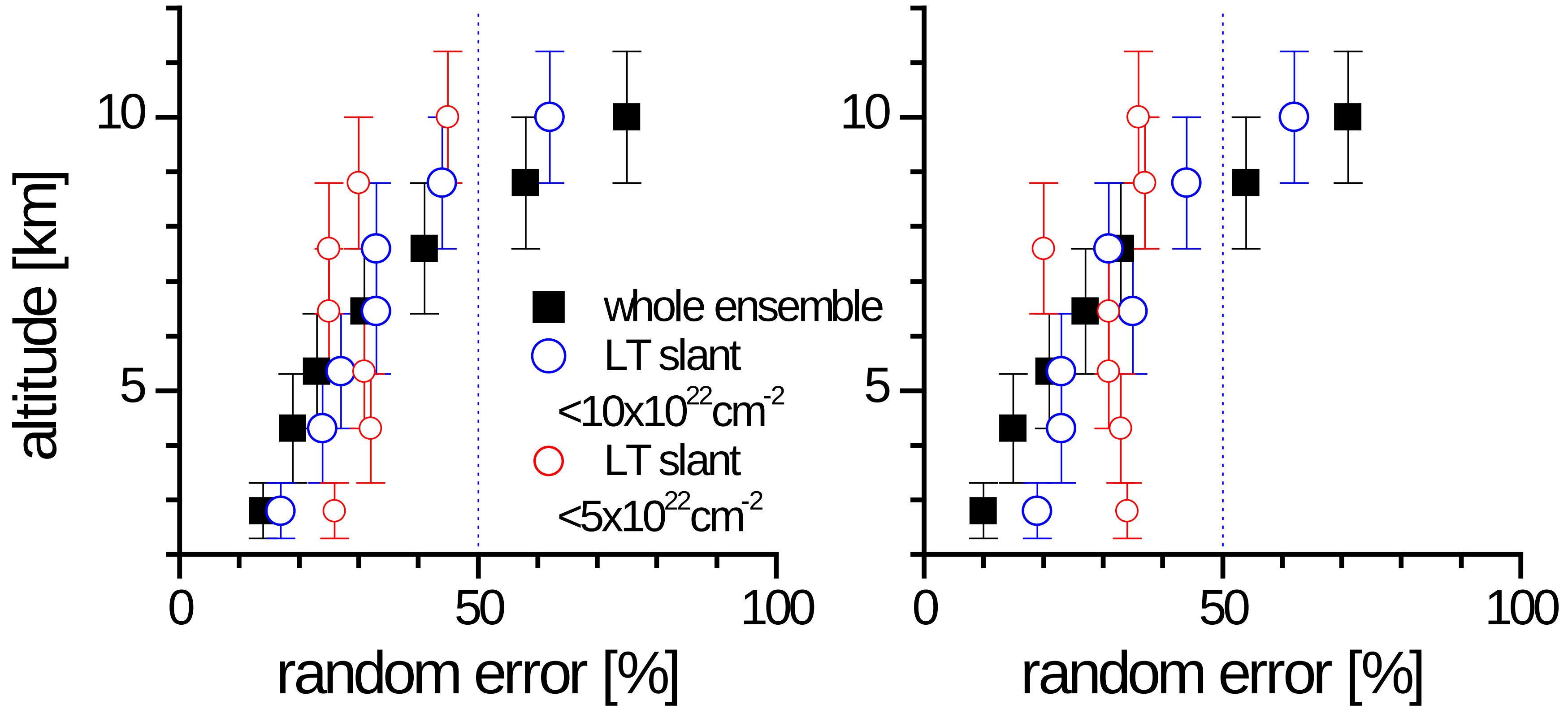
logarithmic scale





Summary of random error component of smoothing + measurement noise error:

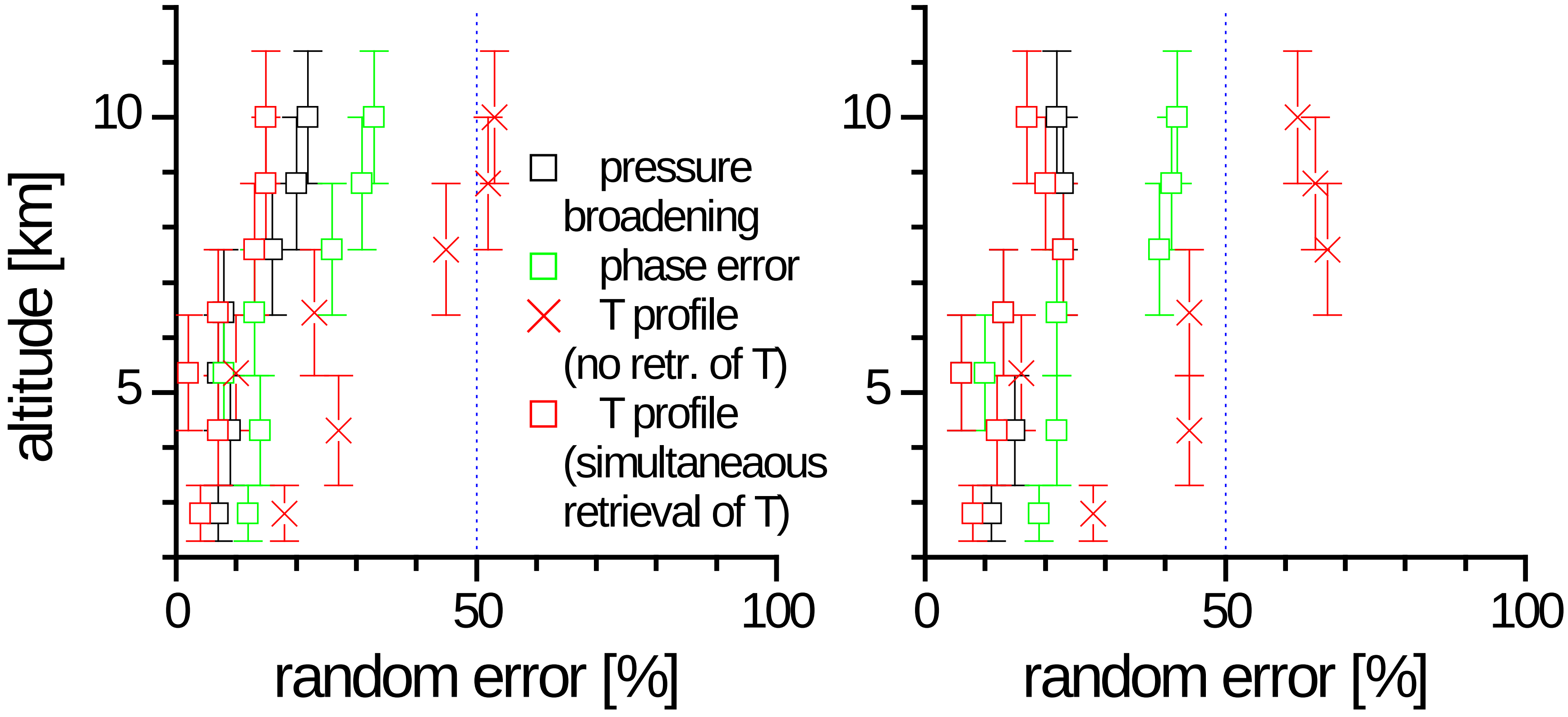
linear scale | logarithmic scale



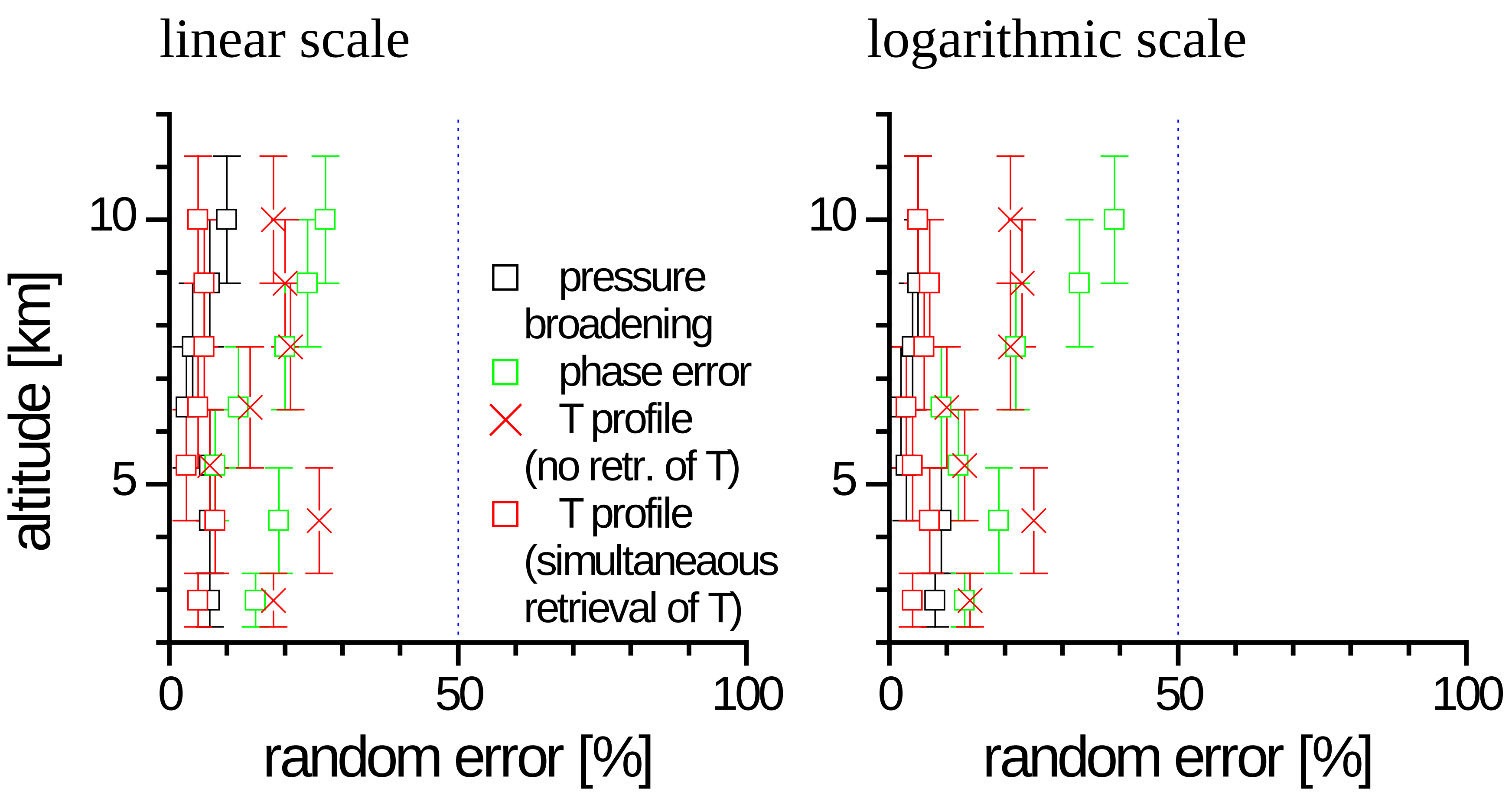
Summary of random error component parameter error (whole ensemble):

linear scale

logarithmic scale



Summary of random error component parameter error (LT slant below 10 x 10^{21}cm^{-1}):



Summary of random error component parameter error (LT slant below 5 x $10^{21}cm^{-1}$

linear scale

logarithmic scale